V I T A

D E N N I S S. M A R Y N I C K

Jenkins Garrett Professor of Chemistry Emeritus
Department of Chemistry and Biochemistry, Box 19065
The University of Texas at Arlington
Arlington, Texas 76019
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EDUCATION

California State University Los Angeles, California	B. S. with Honors in Chemistry, June 1969
Harvard University Cambridge, Massachusetts	M. A. in Chemistry, March 1971 Ph. D. in Chemistry, June 1973 Thesis supervisor: Prof. W. N. Lipscomb

ACADEMIC/RESEARCH POSITIONS HELD

1969-1972	*National Science Foundation Predoctoral Fellow*, Harvard University
1972	*Research Associate*, IBM, San Jose, California
1973	*Research Assistant,* Harvard University
1973-1975	*Miller Institute for Basic Research in Science Fellow,* University of California at Berkeley
1975-1978	*Lecturer and Research Fellow,* Harvard University
1978-1982	*Assistant Professor*, The University of Texas at Arlington
1982-1986	*Associate Professor*, The University of Texas at Arlington
1986-2007	*Professor*, The University of Texas at Arlington
1996-2007	*Jenkins Garrett Professor*, The University of Texas at Arlington

AWARDS AND HONORS

- "Science Teacher of the Year," The University of Texas at Arlington, 1979-80.
- Wilfred T. Doherty Award of the American Chemical Society, Dallas-Fort Worth Section, 1988.
- University Award for Distinguished Research, The University of Texas at Arlington, 1988.
- Jenkins Garrett Professorship, The University of Texas at Arlington, 1996.

SOCIETIES

American Chemical Society
Phi Kappa Phi Honor Society
Sigma Xi
American Association for the Advancement of Science

RESEARCH FUNDING

Robert A. Welch Foundation: "Theoretical Studies of Inorganic Molecules," 6/1/79-5/31/82, $54,000
Organized Research Fund: (The University of Texas at Arlington) Summer Stipend (full), 1980
Organized Research Fund: (The University of Texas at Arlington): "Theoretical Studies of Bonding in Transition Metal Complexes," 9/1/79-8/31/80, $3,050
Robert A. Welch Foundation: "Theoretical Studies of Inorganic Molecules," 6/1/82-5/31/85, $57,000
Organized Research Fund: (The University of Texas at Arlington): "Proton Affinities and Vibrational Zero-Point Energies in Simple Water Derivatives," 9/1/81-8/31/82, $2,900
Research Corporation: "Localized Bonding Patterns in Transition Metal Complexes," 5/28/82, $4,400
Organized Research Fund: (The University of Texas at Arlington): Summer Stipend (one-half), 1983
Robert A. Welch Foundation: (supplement), 6/1/82-5/31/85, $10,000
Robert A. Welch Foundation: "Theoretical Studies of Inorganic Molecules," 6/1/85-5/31/88, $75,000
Organized Research Fund: (The University of Texas at Arlington): "Development of Quantum Mechanical Methodologies for Multi-Nuclear Transition-Metal Complexes," 9/1/85-8/31/86, $4,372
Cray Research, Inc.: "Large Scale Quantum Mechanical Calculations on Molecular Systems," 4/1/86-12/31/86, $40,039
Defense Advanced Research Projects Agency: "Electronic and Ionic Transport in Polymers," M. Pomerantz, J. R. Reynolds, K. Rajeshwar, D. S. Marynick and T. D. Shaffer, 9/15/86-8/31/89, $1,885,000
Robert A. Welch Foundation: (supplement), 6/1/86-5/31/88, $10,000
Cray Research, Inc.: "Large Scale Quantum Mechanical Calculations on Molecular Systems," 1/1/87-12/31/87, $40,039
Robert A. Welch Foundation: "Theoretical Studies of Inorganic Molecules," 6/1/88-5/31/91, $90,000
Searle Research and Development: "Development of the PRDDO Methodology," 1/1/89-12/31/89, $10,000
Research Enhancement Program Grant: (The University of Texas at Arlington), 1988, $1,000
Texas Advanced Technology Program: "Advanced Molecular Modeling Software for Quantum Biochemical Applications," D. S. Marynick and S. K. Estreicher, 1/1/90-12/31/91, $127,000
Defense Advanced Research Projects Agency: "Electronic and Ionic Transport in Polymers," M. Pomerantz, J. R. Reynolds, K. Rajeshwar, and D. S. Marynick, 10/1/89-9/30/91, $1,147,000
Cray Research, Inc.: "Molecular Orbital Techniques for Very Large Molecules," 4/1/91-3/31/92, $47,800
Robert A. Welch Foundation: "Theoretical Studies of Inorganic Molecules," 6/1/91-5/31/94, $105,000
National Science Foundation: "Research Experiences for Undergraduates," R. J. Blau, PI with several additional Chemistry Department Faculty, 3/1/91-2/28/94, $113,627
Cray Research, Inc.: "Molecular Orbital Techniques for Very Large Molecules," 1/1/92-12/31/92, $38,000
National Institutes of Health: "Electronic Structure of Vitamin B_{12} and Related Systems," 6/1/92-5/31/95, $108,776

Air Force Office of Scientific Research: "Superconductive Organic Polymers: Conceptual Design, Synthesis, and Characterization" (with R.L. Elsenbaumer, Martin Pomerantz and S.C. Sharma), 1992-1995, $550,000
Cray Research, Inc.: "New Techniques for Mapping Multidimensional Potential Energy Surfaces," 1/1/94-12/31/94, $28,200
Robert A. Welch Foundation: "Electronic Structure Studies on Very Large Molecules," 6/1/94-5/31/97, $111,000
Cray Research, Inc. : "The Electronic Structures of Extremely Large Molecules: Two Important Examples" 1/1/95-12/31/95 $37,500
Robert A. Welch Foundation: "Electronic Structure Studies on Very Large Molecules," 6/1/97-5/31/00, $152,000
Robert A. Welch Foundation: "Electronic Structure Studies on Very Large Molecules," 6/1/00-5/31/03, $180,000
Robert A. Welch Foundation: "Application of Density Functional Theory to Fundamental Issues in Biomolecular and Inorganic Systems," 6/1/03-5/31/06, $200,000
Robert A. Welch Foundation: "Fundamental Computational Studies of Gas Phase Ion-Molecule Chemistry, 6/1/06-5/31/09, $240,000

PAPERS PRESENTED

"*Ring Current Calculations and NMR Chemical Shifts in Pyramidal Boron Hydrides and Carboranes*," National Meeting of the American Chemical Society, Atlantic City, New Jersey, September 1968.

"*The Crystal and Gas Phase Structure of Beryllium Borohydride*," California State University at Los Angeles, January 1973.

"*Some Mathematical Aspects of Localized Orbital Calculations*," University of California at Berkeley, December 1974.

"*A Theoretical Study of Metal-Phosphate Complexes*," University of California at Los Angeles, December 1974.

"*Localized Orbitals in Boranes and Carboranes. The Edmiston-Ruedenberg Approach*," Second International Meeting on Boron Chemistry, Leeds, England, March 1984.

"*A Theoretical Study of Metal-Phosphate Complexes*," Institut de Chemie, Universite Louis Pasteur, Strasbourg, France, April 1975.

"*What is the Structure of Beryllium Borohydride?*," Institut de Chemie, Universite Louis Pasteur, Strasbourg, France, April 1975.

"*Theoretical Aspects of Beryllium Chemistry*," University of Michigan, May 1975.

"*What is the Structure of Beryllium Borohydride?*," University of Illinois, May 1976.

"*Some Aspects of Molecular Electronic Structure Theory*," The University of Texas at Arlington, April 1977.

"*Development and Application of Approximate Molecular Orbital Calculations*," The University of Texas at Arlington, March 1979.

"*Inversion Barriers of Molecules with General Formula AX_3*," National Meeting of the American Chemical Society, Houston, Texas, March 1980.

"*Two Problems in Theoretical Inorganic Chemistry*," Texas Christian University, November 1980.

"*The Electron Pair Bond in Transition Metal Complexes*," The University of Texas at Arlington, April 1981.

"*Computer Chemistry*," Bishop College, November 1982.

"*Theoretical Studies of Transition Metal Complexes*," The University of Arkansas, March 1983.

"*Theoretical Studies of Transition Metal Complexes*," Morehouse College, March 1983.

"*Theoretical Studies of Transition Metal Complexes*," Auburn University, March 1983.

"*Theoretical Studies of Transition-Metal Complexes*," Southern Methodist University, May 1983.

"*Cis-Trans Isomerism and Pi Bonding in Transition-Metal Complexes. A Theoretical Study,*" Tenth Austin Symposium on Molecular Structure, The University of Texas at Austin, February 1984.

"*Theoretical Organometallic Chemistry*," University of Texas at Dallas, February 1984.

"*Theoretical Organometallic Chemistry*," Stephen F. Austin University, March 1984.

"*Structure, Conformation and Localized Bonding Patterns in Transition-Metal Complexes*," Robert A. Welch Foundation on Chemical Research XXVIII, November 1984.

"*Approximate Molecular Orbital Studies on Transition-Metal Complexes*," Searle Research and Development, Chicago, Illinois, July 1985.

"*The Quantum Mechanics of Molecular Systems: Methodology and Application*," Rice University, February, 1986.

"*Theoretical Organometallic Chemistry*," Texas Tech University, October 1986.

"*Theoretical Studies of Group Migrations in Pentacarbonyl(alkyl)manganese(I) Systems*," D. S. Marynick and F. U. Axe, 192nd Meeting of the American Chemical Society, Anaheim, California, September 1986.

"*Theoretical Organometallic Chemistry*," University of Oklahoma, February 1987.

"*Structural Control of the Electronic and Ionic Properties of Polyheterocycles*," S. Basak, D. Black, D. S. Marynick, T. Pajkossy, M. Pomerantz, P. A. Poropatic, K. Rajeshwar, J. R. Reynolds, N. Sundaresan, and R. Toyooka, 193rd Meeting of the American Chemical Society, Denver, Colorado, April 1987.

"*Electronic Structure Studies of Heteroatomic Zintl Anions* ," F. U. Axe and D. S. Marynick, 193rd Meeting of the American Chemical Society, Denver, Colorado, April 1987.

"Three Problems in Theoretical Organometallic Chemistry," North Texas State University, May, 1987.

"*Dirac Scattered Wave Study of* $PaCl_6^{2-}$," R. Arratia-Perez and D. S. Marynick, 194th Meeting of the American Chemical Society, New Orleans, LA, August, 1987.

"*Theoretical Study of the Direct Insertion Mechanism in Ziegler-Natta Polymerization*," C. A. Jolly and D. S. Marynick, 194th Meeting of the American Chemical Society, New Orleans, LA, August, 1987.

"*Theoretical Calculations of the Fluxional Behavior of the Cyclopentadienyl Ligand in Titanium(IV) Complexes*," L. Hanson and D. S. Marynick, 194th Meeting of the American Chemical Society, New Orleans, LA, August, 1987.

"*Potential Energy Surfaces in Real Organometallic Systems*," University of Texas at El Paso, October, 1987.

"Chemistry without Chemicals," The University of Texas at Arlington, A.C.S. Student Affiliates, December, 1987.

"*Probing Chemistry with Quantum Mechanic*s," Dallas-Fort Worth Section of the American Chemical Society, The University of Texas at Arlington, April, 1988 (Wilfred T. Doherty Award Lecture).

"*Electronic Structure Calculations on Large Organometallic Systems*," Second International Conference on Computational Chemistry on Cray Supercomputers, Chicago, Illinois, September, 1988.

"Theoretical Studies of Organometallic Reaction Mechanisms," University of Calgary, January, 1989.

"Exploring Organometallic Reaction Mechanisms from a Theoretical Perspective," Searle Research and Development, Chicago, Illinois, January, 1989.

"PRDDO: Methodology and Application," Cray Research, Inc., Mendota Heights, Minnesota, March, 1989.

"Localized Bonding Patterns in Zintl Anions," M. Jackson and D. S. Marynick, 197th Meeting of the American Chemical Society, Dallas, Texas, April, 1989.

"A Theoretical Study of the Cis-Trans Intramolecular Isomerization Mechanism in $Cr(CO)_5R$, R=CO, PH_3 and PPh_3," L. M. Hansen and D. S. Marynick, 197th Meeting of the American Chemical Society, Dallas, Texas, April, 1989.

"Electronic Structures of a Series of Polyatomic Zintl Anions: Bi_4^{2-}, Sb_4^{2-}, and Sb_7^{2-}. A Scattered Wave X-α Study," C. A. Jolly and D. S. Marynick, 197th Meeting of the American Chemical Society, Dallas, Texas, April, 1989.

"A Molecular Orbital Study of Methyl Migration in Tetracarbonyl(methyl)cobalt(I)," J. R. Rogers and D. S. Marynick, 197th Meeting of the American Chemical Society, Dallas, Texas, April, 1989.

"Chemical Bonding in Really Strange Molecules," The University of Texas at Arlington, April, 1989.

"Theoretical Studies of Organometallic Reaction Mechanisms," California State University at Los Angeles, April, 1989.

"Organometallic Reaction Mechanisms: A Theoretical Perspective," West Texas State University, University of Texas at San Antonio, University of Dallas; March, 1990.

"*Theoretical Perspectives on Structure and Reactivity in Organometallic Systems,"* Harvard University, June, 1990.

"*Computer Chemistry*," Midwestern State University, March 1991.

"*Computer Chemistry*," University of Texas at Arlington, March 1991.

"*Electronic and Conformational Interplay in C_2X_4–Bridged Bimetallic Complexes,*" Jimmy R. Rogers, Chad K. Johnson, and D. S. Marynick, Southwest Theoretical Chemistry Conference, Dallas, Texas, November, 1991.

"*Modified Extended Hückel Band Calculations on Conjugated Polymers*," S. Y. Hong and D. S. Marynick, Southwest Theoretical Chemistry Conference, Dallas, Texas, November, 1991.

"*Inclusion of Frozen Core Potentials into the Method of Partial Retention of Diatomic Differential Overlap (PRDDO)*," A. Derecskei-Kovacs, D. E. Woon and D. S. Marynick, Southwest Theoretical Chemistry Conference, Dallas, Texas, November, 1991.

"*Electronic and Conformational Interplay in C_2X_4-Bridged Bimetallic Complexes,*" J. R. Rogers, C. Johnson and D. S. Marynick, Southwest Theoretical Chemistry Conference, Dallas, Texas, November, 1991.

"*Modified Extended Hückel Band Calculations on Conjugated Polymers,*" S. Y. Hong and D. Marynick, Southwest Theoretical Chemistry Conference, Dallas, Texas, November, 1991.

"*Frozen Core Potentials in the Method of Partial Retention of Diatomic Differential Overlap,*" A. Derecskei-Kovacs, D. E. Woon and D. S. Marynick, Sanibel Symposia, March, 1992.

"*Understanding the Conformational Stability and Electronic Structure of Modified Polymers Based on Polythiophene,*" D. S. Marynick and S. Y. Hong, 103rd Meeting of the American Chemical Society, San Francisco, California, April, 1992.

"*To Polymerize or Not To Polymerize: That is the Question,*" J. R. Reynolds and D. S. Marynick, 103rd Meeting of the American Chemical Society, San Francisco, California, April, 1992.

"*Exploring Potential Energy Surfaces in Organometallic Systems,*" University of Houston, April, 1992.

"*Chemistry in the Computer,*" New Mexico University of the Highlands, February, 1993.

"*Exploring Potential Energy Surfaces in Organometallic Systems,*" University of North Texas, April, 1993.

"*Electronic Structure of Very Large Molecules: The PRDDO/M Method*," Swiss Center for Scientific Computing, Lugano, Italy, July, 1993.

"*Computer Chemistry*," Pittsburgh State University, April, 1994.

"*Very Large Scale Molecular Orbital Calculations on Biomolecules: From Vitamin B_{12} to Cytochrome c and Beyond,*" Instituto di Richerche di Biologia Molecolare P. Angeletti SpA (IRBM), Rome, Italy, July, 1994.

"*Pushing Molecular Quantum Mechanics to the Limit: The PRDDO/M Method,*" Swiss Center for Scientific Computing, Lugano, Italy, July, 1994.

"*Approximate ab initio Calculations on Very Large Molecules,*" International Workshop on Electronic Structure Methods for Truly Large Systems: Moving the Frontiers in Quantum Chemistry, Brunlage, Germany, August, 1994.

"*Conformational Analysis of Tetrathiafulvalene Isomers and the Band Structure of Their One Dimensional Polymers,* " D. S. Marynick and S. Seong, Southwest regional ACS meeting, Ft. Worth, Tx., Nov., 1994.

"*Electronic Structure Calculations on Extremely Large Molecules,*" University of Denver, Feb., 1995.

"*Electronic Structure Calculations on Extremely Large Molecules,* Colorado School of Mines, Jan., 1995.

"*Computer Chemistry,*" East Texas State University, March, 1995.

"*Chemistry Without Chemicals: Computational Modeling of Chemical Phenomena*", Arkansas Tech University and Henderson State University, November, 1995.

"*Combined Ab Initio-Density Functional Study of Difficult Problems in Structural Inorganic Chemistry*," Pacifichem '95, Honolulu, Hawaii, December, 1995.

"*Electronic Structure Studies of Very Large Inorganic Systems*," Symposium on Computational Advances in Inorganic Chemistry, Division of Computers in Chemistry, 212th National Meeting of the American Chemical Society, Orlando Fl, Aug., 1996.

"*The Quantum Mechanics of Very Large Molecules*," University of Texas at El Paso, Oct., 1996.

"*The Quantum Mechanics of Very Large Molecules*," University of Texas at Arlington, Oct., 1996.

"*Accurate Molecular Electrostatic Potentials for Very Large Molecules*," Southwest Theoretical Chemistry Conference, Arlington, TX, Nov., 1996.

"*Industrial Internships and the Ph.D. in Applied Chemistry at the University of Texas at Arlington*," R. L. Elsenbaumer, D. S. Marynick, G. R. Kinsel and A. L. Ternay, 225th Meeting of the American Chemical Society, March, 1998.

"*Quantum Mechanical Study of Polarization Effects on Enzyme-Substrate Interactions*," D. S. Marynick and J. H. Wu, 225th Meeting of the American Chemical Society, March, 1998.

"*Ab Initio DFT Study of the Gas-Phase Proton Affinity of Glutamic Acid*," W. Sun, D. S. Marynick and G. R. Kinsel, 225th Meeting of the American Chemical Society, March, 1998.

"*Conformational Preferences in C_2X_4 Bridged Bimetallic Transition-Metal Complexes*," L. W. Mire and D. S. Marynick, 225th Meeting of the American Chemical Society, March, 1998.

"*On the nature of the Long-Lived Transient in the Photodecarbonylation of $Mn(CO)_5CH_3$: The Energetic Consequences of Agostic and Dihapto Stabilization in $Mn(CO)_5C(O)CH_3$*." A. Derecskei-Kovacs and D. S. Marynick, 225th Meeting of the American Chemical Society, Anaheim, CA. March, 1998.

"*The Structures of Small Silver Bromide Clusters*," H. Zhang, Z. A. Schelly and D. S. Marynick, Southwest Theoretical Chemistry Conference, Denton, TX. Nov. 1998.

"*Industrial internships and the Ph.D in applied chemistry at the University of Texas at Arlington,"* Elsenbaumer, Ronald L.; Marynick, Dennis S.; Kinsel, Gary R.; Ternay, Andrew L., Jr. 215th ACS National Meeting, Dallas, March 29-April 2 (1998)

"Computational study of ionization potentials and proton transfer in small clusters of 2,5-dihydroxybenzoic acid," E.F. Archibong, G.R. Kinsel and D.S. Marynick, 227th Meeting of the American Chemical Society, New Orleans, LA. August, 1999.

"Are fullerenes and carbon nanotubes viable candidates for η^6 metal ligands?" S. K. Goh, D.S. Marynick, 227th Meeting of the American Chemical Society, New Orleans, LA. August, 1999.

"*The Migration-Insertion Reaction*," Texas Tech University, October, 1999.

"Two Problems in Computational Organometallic Chemistry," University of Florida, October, 1999.

"The Migration/Insertion Reaction," U. T. Arlington, November, 1999.

"*A New Look at an Old Reaction: Methyl Migration in Pentacarbonyl(methyl)manganese(I),*" University of North Texas, November, 2000.

"Preparation of Quantum Dots via Electroporation of Vesicles," Z. A. Schelly, N. M. Correa, H. Zhang, D. S. Marynick: Invited Paper at 'Particles 2001', February, 2001, Orlando, Florida.

"Gas-Phase Models of Enzyme-Substrate Interactions. The Effects of Hydrogen-Bonding Interactions on Substrate Ionization Potentials," D. S. Marynick, G. R. Kinsel, S.-K. Goh, E. F. Archibong and J. Hardesty, 222th Meeting of the American Chemical Society, Chicago, Il. August, 2001.

"CdS Quantum Dots Prepared via Electroporation of Vesicles: Experimental and Computational Results." H. Zeng, D. S. Marynick and Z. A. Schelly, 225th ACS National Meeting, March, 2003, New Orleans, LA.

"*Thermodynamic properties of MALDI matrices*," F. Yassin and D. S. Marynick, 227th ACS National Meeting, Anaheim, CA, United States, March, 2004.

"Modeling Molecular Interaction in MALDI Mass Spectrometry," D. S. Marynick, 228th ACS National Meeting, Philadelphia, United States, August, 2004.

"Computational Estimates of the Gas-Phase Basicities, Proton Affinities and Ionization Potentials of the Six Isomers of Dihydroxybenzoic Acid," F. H. Yassin and D. S. Marynick, 228th ACS National Meeting, Philadelphia, United States, August, 2004.

"Computational studies of MALDI matrices interacting with tripeptides as a model of MALDI matrix-analyte interactions," F. H. Yassin and D. S. Marynick, 228th ACS National Meeting, Philadelphia, United States, August, 2004.

"Experimental and Computational Studies of Equilibrium Conditions in MALDI Plumes," Gary R. Kinsel, Daqing Yao, Faten Yassin and Dennis S. Marynick, Desorption 2004, Saint-Petersburg, Russia, Sept, 2004.

"*Ionization Potentials of Matrix-Peptide Clusters in MALDI Mass Spectrometry,* " Dennis S. Marynick, Faten H. Yassin, Jayakumar Narayanasamy, Kaori Noto and Gary R. Kinsel, Southwest Regional Meeting of the American Chemical Society, Ft. Worth, Texas, Sept., 2004.

"*Modeling Molecular Interactions in MALDI Mass Spectrometry*," Symposium in Honor of William N. Lipscomb's 80th Birthday," Shanghai, China, August 2005.

"*Modeling Molecular Interactions in MALDI Mass Spectrometry*," Texas Tech University, March, 2007

PUBLICATIONS

1. "Ring Current Calculations and Proton Nuclear Magnetic Resonance Chemical Shifts in 2,3-Dicarbahexaborane(8) and Some Derivatives," T. Onak, D. Marynick and P. Mattschei, *Chem. Comm.*, 557-558 (1968).

2. "The Preparation of B-Methyl Derivatives of $C_2B_4H_8$. The Correlation of Proton Nuclear Magnetic Resonance Chemical Shifts in $C_2B_4H_8$ Derivatives by Employing 'Ring-Current' Contributions," T. Onak, D. Marynick, P. Mattschei and G. Dunks, *Inorg. Chem.*, **7**, 1754-1757 (1968).

3. "A Correlation of Nuclear Magnetic Resonance Chemical Shifts in Pyramidal Boron Compounds Using a Conical Ring Current Model," D. Marynick and T. Onak, *J. Chem. Soc.*, Section A, 1797-1801 (1969).

4. "Low Temperature and Paramagnetic Ion Effects on the Proton and Boron-11 Nuclear Magnetic Resonance Spectra of the Triborohydride Ion ($B_3H_8^-$)," D. Marynick and T. Onak, *J. Chem. Soc.*, Section A, 1160-1161 (1970).

5. "Application of a Ring Current Model to Decaborane(14)," T. Onak and D. Marynick, *Tran. Faraday Soc.*, **66**, 1843-1847 (1970).

6. "Beryllium Borohydride Structure in the Solid Phase," D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **93**, 2322-2323 (1971).

7. "Convergence in Orbital Localization Procedures," D. S. Marynick and E. Switkes, *Chem. Phys. Lett.*, **15**, 133-135 (1972).

8. "Crystal Structure of Beryllium Borohydride," D. S. Marynick and W. N. Lipscomb, *Inorg. Chem.*, **11**, 820-823 (1972).

9. "Fractional Three-Center Bonds in Carboranes," D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **94**, 1748-1750 (1972).

10. "*Ab initio* Self-Consistent Field Calculation of the Energies of Formation of B_2H_6 and $B_2H_7^-$," J. H. Hall, Jr., D. S. Marynick and W. N. Lipscomb, *Inorg. Chem.*, **11**, 3126-3128 (1972).

11. "A Self-Consistent Field and Localized Orbital Study of 4,5-Dicarbahexaborane(8)," D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **94**, 8699-8706 (1972).

12. "Self-Consistent Field Wavefunction and Localized Orbitals for 2,4-Dicarbaheptaborane(7). The Fractional Three-Center Bond," D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **94**, 8692-8699 (1972).

13. "Localized Molecular Orbitals for 1,2- and 1,6-Dicarbahexaborane(6). The Open Three-Center Bond, and Implications for Carborane Topology," I. R. Epstein, D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **95**, 1760-1766 (1973).

14. "*Ab initio* Self-Consistent Field and Configuration Interaction Study of Beryllium Borohydride," D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **95**, 7244-7250 (1973).

15. "Self-Consistent Field Wave Functions of Boron Hydrides and Ions: B_8H_{12}, B_9H_{15}, $B_6H_6^{2-}$, $B_{10}H_{10}^{2-}$, and $B_{10}H_{14}^{2-}$," J. H. Hall, Jr., D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **96**, 770-779 (1974).

16. "Energy of Formation of Diborane Near the Hartree-Fock Limit," D. S. Marynick, J. H. Hall, Jr. and W. N. Lipscomb, *J. Chem. Phys.*, **61**, 5460-5461 (1974).

17. "One Electron Properties of Phosphine Calculated from Self-Consistent Field Wavefunctions," J. H. Hall, Jr., D. S. Marynick, D. A. Dixon, B. F. P. Edwards and W. N. Lipscomb, *Proc. Soc. Black Chemists and Chemical Engineers*, Vol. **1**, Ch. 12, p. 1-7 (1975).

18. "A Mathematical Treatment of Rate Data Obtained in Biological Flow Systems Under Nonsteady State Conditions," D. S. Marynick and M. C. Marynick, *Plant Physiol.*, **56**, 680-683 (1975).

19. "Theoretical Studies of Metal-Phosphate Interactions: Interactions of Li^+, Na^+, Be^{++}, Mg^{++} and Ca^{++} with $H_2PO_4^-$ and $(CH_3O)_2PO_2^-$: Implications for Nucleic Acid Solvation," D. S. Marynick and H. F. Schaefer, III, *Proc. Nat. Acad. Sci. USA*, **72**, 3794-3798 (1975).

20. "The Synthesis and Properties of 2-Chloro-1,6-Dicarbahexaborane(6)," J. R. Spielman, R. Warren, D. A. Bergquist, J. K. Allen, D. Marynick and T. Onak, *Synthesis and Reactivity in Inorganic and Metalorganic Chemistry*, **5**, 347-356 (1975).

21. "NMR Coupling, Hybrid Orbital Character, and Bond Distances in the Boron Hydrides," T. Onak, J. Leach, S. Anderson, M. J. Frisch and D. S. Marynick, *J. Mag. Res.*, **23**, 237-248 (1976).

22. "Beryllium Borohydride: C_{3v} or D_{3d}?," D. S. Marynick, *J. Chem. Phys.*, **64**, 3080-3081 (1976).

23. "Theoretical Studies of Inversion Barriers in Pyramidal Molecules," D. S. Marynick and D. A. Dixon, *Disc. Faraday Soc.*, **62**, 47 (1976).

24. "*Ab initio* Self-Consistent Field Studies of Metal-Phosphate Complexes," D. S. Marynick, *J. Mol. Structure*, **36**, 339-342 (1977).

25. "Studies of the Molecular and Electronic Structure of Dicyclopentadienylberyllium," D. S. Marynick, *J. Am. Chem. Soc.*, **99**, 1436-1441 (1977).

26. "The Electron Affinity of the Methyl Radical. The Structure of CH_3 and CH_3^-," D. S. Marynick and D. A. Dixon, *Proc. Nat. Acad. USA*, **74**, 410-413 (1977).

27. "The Inversion Barriers of AsH_3 and SeH_3^+," D. A. Dixon and D. S. Marynick, *J. Am. Chem. Soc.*, **99**, 6101-6103 (1977).

28. "Basis Set and Electron Correlation Effects on the Total Electron Density in H_2O, H_2S, and BH," J. Bicerano, D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **100**, 732-739 (1978).

29. "Large Closo Boron Hydrides," J. Bicerano, D. S. Marynick and W. N. Lipscomb, *Inorg. Chem.*, **17**, 2040 (1978).

30. "Estimate of the Inversion Barrier in SbH_3," D. S. Marynick and D. A. Dixon, *J. Chem. Phys.*, **69**, 498-500 (1978).

31. "Molecular Orbital Studies on Large Closo Boron Hydrides," J. Bicerano, D. S. Marynick and W. N. Lipscomb, *Inorg. Chem.*, **17**, 3443-3453 (1978).

32. "Tautomerism in Monocarbahexaborane(7)," S. K. Lambiris, D. S. Marynick and W. N. Lipscomb, *Inorg. Chem.*, **17**, 3706-3707 (1978).

33. "Classical Configurations Associated with Non-Classical Molecules," R. N. Camp, D. S. Marynick, G. D. Graham and W. N. Lipscomb, *J. Am. Chem. Soc.*, **100**, 6781-6783 (1978).

34. "Ligand Exchange in Tax (η^4-naphthalene)$(Me_2PC_2H_4PMe_2)_2$: The Pentagonal Bipyramid to Monocapped Trigonal Prism Traverse," J. O. Albright, S. Datta, B. Dezube, J. K. Kouba, D. S. Marynick and S. S. Wreford, *J. Am. Chem. Soc.*, **101**, 611-619 (1979).

35. "Model Studies of the Electronic Structure of Solid State Beryllium Borohydride," D. S. Marynick, *J. Am. Chem. Soc.*, **101**, 6876-6880 (1979).

36. "The Geometry and Inversion Barrier of the Sulfonium Ion SH_3^+. Dependence on Basis Set," D. A. Dixon and D. S. Marynick, *J. Chem. Phys.*, **71**, 2860-2863 (1979).

37. "A Theoretical Study of the Structure and Inversion Barrier of PLi_3," D. S. Marynick, *Chem. Phys. Lett.*, **75**, 550-552 (1980).

38. "The Proton Affinity of Ammonia. A Theoretical Determination," R. A. Eades, K. Scanlon, M. R. Ellenberger, D. A. Dixon and D. S. Marynick, *J. Phys. Chem.*, **84**, 2840-2842 (1980).

39. "Isomers of Dicarbaclosopentaborane(5) and Their Methyl and Fluoro Derivatives. A Theoretical Study," G. D. Graham, D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **102**, 2939-2945 (1980).

40. "Calculated Inversion Barrier of AsF_3," D. S. Marynick, *Chem. Phys. Lett.*, **71**, 101-103 (1980).

41. "The Inversion Barriers of NF_3, NCl_3, PF_3, and PCl_3. A Theoretical Study," D. S. Marynick, *J. Chem. Phys.*, **73**, 3939-3943 (1980).

42. "The Effects of Basis Set and Configuration Interaction on the Electronic Structure of Methyl Lithium with Comments on the Nature of the C-Li Bond," G. D. Graham, D. S. Marynick and W. N. Lipscomb, *J. Am. Chem. Soc.*, **102**, 4572-4578 (1980).

43. "An SCF-CI Study of the Structures, Inversion Barriers, and Inversion Frequencies of SiH_3, PH_3^+, and SH_3^{++}," D. S. Marynick, *J. Chem. Phys.*, **74**, 5186-5189 (1981).

44. "A Molecular Orbital Study of Hydrogen, Methyl, and Phenyl Bridging in Beryllium Compounds," D. S. Marynick, *J. Am. Chem. Soc.*, **103**, 1328-1333 (1981).

45. "Absolute Proton Affinities of PH_3 and H_2S," D. S. Marynick, K. Scanlon, R. A. Eades and D. A. Dixon, *J. Phys. Chem.*, **85**, 3364-3366 (1981).

46. "A Molecular Orbital Study of Cyanide Complexes of BX_3 and AlX_3, X = H, CH_3, F, and Cl," D. S. Marynick, L. Throckmorton and R. Bacquet, *J. Am. Chem. Soc.*, **104**, 1-5 (1982).

47. "A Theoretical Study of the Structures and Inversion Barriers of CF_3^- and SiF_3^-," D. S. Marynick, *J. Mol. Struct.*, **87**, 161-168 (1982).

48. "Extension of the Method of Partial Retention of Diatomic Differential Overlap to Second Row Atoms and Transition Metals," D. S. Marynick and W. N. Lipscomb, *Proc. Nat. Acad. Sci. U.S.A.*, **79**, 1341-1345 (1982).

49. "Determination of *Ab initio* Force Constants of F_2O and H_2O," D. S. Marynick and C. V. S. Rao, *Chem. Phys. Lett.*, **86**, 307-311 (1982).

50. "The Electronic Structure of PH_3. The Effect of Basis Set and Correlation on the Inversion Barrier," D. S. Marynick and D. A. Dixon, *J. Phys. Chem.*, **86**, 914-917 (1982).

51. "On the Electronic Structure of Planar Fluorinated Amines and Phosphines," D. S. Marynick, D. C. Rosen and J. F. Liebman, *J. Mol. Struct.*, **94**, 47-50 (1983).

52. "Localized Molecular Orbital Studies of Transition Metal Complexes. I. Simple Octahedral Complexes of General Formula $(NH_3)_5M$-L, M = Sc^{3+}, Cr, Mn^+, Fe^{2+}, Co^{3+}, or Zn^{2+}, and L = H^-, NH_3, CH_3^-, F^-, Cl^-, or H_2O," D. S. Marynick and C. M. Kirkpatrick, *J. Phys. Chem.*, **87**, 3273-3279 (1983).

53. "Theoretical Estimates of the Proton Affinities of OLi_2, OF_2, and OCl_2," D. S. Marynick and D. A. Dixon, *J. Phys. Chem.*, **87**, 3430-3433 (1983).

54. "C-13 and P-31 NMR Studies of ^{13}CN-Cyanocobalamin in Sulfuric Acid-Water Mixture," K. L. Brown, J. M. Hakimi and D. S. Marynick, *Inorg. Chim. Acta*, **79**, 120-122 (1983).

55. "Equilibrium Geometries of Transition Metal Complexes. A Comparison of Approximate Molecular Orbital Theory and Experiment," D. S. Marynick, F. U. Axe, C. M. Kirkpatrick and L. Throckmorton, *Chem. Phys. Lett.*, **99**, 406-410 (1983).

56. "The Electronic Structure of Nitromethane. A Multiconfiguration Self-Consistent Field Study," D. S. Marynick, A. K. Ray, J. L. Fry and D. A. Kleier, *J. Mol. Struct., THEOCHEM*, **108**, 45-48 (1984).

57. "Structure, Conformation, and Ligand Binding in $Fe(CO)_4(C_2H_4)$ and Some Derivatives. A Theoretical Study," F. U. Axe and D. S. Marynick, *J. Am. Chem. Soc.*, **106**, 6230-6235 (1984).

58. "Pi Accepting Abilities of Phosphines in Transition Metal Complexes," D. S. Marynick, *J. Am. Chem. Soc.*, **106**, 4064-4065 (1984).

59. "Localized Valence Structures of Transition-Metal Carbene Complexes," D. S. Marynick and C. M. Kirkpatrick, *J. Am. Chem. Soc.*, **107**, 1993-1994 (1985).

60. "A Theoretical Study of Cis-Trans Isomerization in Simple Transition Metal Complexes," D. S. Marynick, S. Askari and D. F. Nickerson, *Inorg. Chem.*, **24**, 868-870 (1985).

61. "Localized Molecular Orbital Studies of Transition Metal Complexes. II. Pi Accepting Ligands," C. M. Kirkpatrick and D. S. Marynick, *J. Comput. Chem.*, **6**, 142-147 (1985).

62. "Electronic Structure Calculations on R-NO_2 Species, R = H, CH_3, NH_2, HO and F," D. S. Marynick, A. K. Ray and J. L. Fry, *Chem. Phys. Lett.*, **116**, 429-433 (1985).

63. "Mechanism of Acid-Induced Decomposition of 2-Hydroxyethyl- and 2-Alkoxyethyl-cobaloximes," K. L. Brown, S. Ramamurthy and D. S. Marynick, *J. Organomet. Chem.*, **287**, 377-394 (1985).

64. "Surface Effects in Cluster Calculations of Energy Profiles of Mu in Diamond," S. Estreicher, A. K. Ray, J. L. Fry and D. S. Marynick, *Phys. Rev. Lett.*, **55**, 1976-1978 (1985).

65. "Systematic Errors in the Total Energy of Molecular Wavefunctions Calculated within the PRDDO Approximations," L. Throckmorton and D. S. Marynick, *J. Comput. Chem.*, **6**, 652-656 (1985).

66. "Structure, Conformation and Localized Bonding Patterns in Transition Metal Complexes," D. S. Marynick, *Proceedings of the Robert A. Welch Foundation Conference on Chemical Research XXVIII*, Houston, Texas, 1984 (published in 1986).

67. "A Comparison of Calculated and Experimental Metal-Ligand Bond Lengths in Early Transition-Metal Complexes Using the Method of Partial Retention of Diatomic Differential Overlap," D. S. Marynick and R. D. Reid, *Chem. Phys. Lett.*, **124**, 17-19 (1986).

68. "NMR Spectroscopy and Cyclic Voltammetry of N-Aryl-*P,P,P*-triphenyl-λ5-azenes. Substituent Effects and Correlation with Molecular Orbital Calculations," M. Pomerantz, D. S. Marynick, K.

Rajeshwar, W. Chou, L. Throckmorton, E. W. Tsai, P. C. Y. Chen and T. Carr, *J. Org. Chem.*, **51**, 1223-1230 (1986).

69. Comment on "Identification of Anomalous Muonium in Semiconductors as a Vacancy Associated Center by N. Sahoo, K. C. Mishra and T. P. Das, *Phys. Rev. Lett.*, **55**, 1506 (1985)," E. Estreicher and D. S. Marynick, *Phys. Rev. Lett.*, **56**, 1511 (1986).

70. "Electrochemistry of Thioxanthene, Thioxanthane, and Related Compounds in Acetonitrile. Substituent Effects and Correlation with Molecular Orbital Calculations," E. W. Tsai, L. Throckmorton, R. McKellar, M. Barr, M. Kluba, D. S. Marynick, K. Rajeshwar and A. L. Ternay, *J. Electroanalytical Chem.*, **210**, 45-67 (1986).

71. "Interstitial Hydrogen in Diamond: A Detailed Hartree-Fock Analysis," S. Estreicher, A. K. Ray, J. L. Fry, and D. S. Marynick, *Phys. Rev. B.*, **34**, 6071-6079 (1986).

72. "Lattice Relaxations for Normal Muonium in Diamond," S. Estreicher and D. S. Marynick, *Hyperfine Inter.*, **32**, 613-617 (1986).

73. "Preliminary Calculation Confirming that Anomalous Muonium in Diamond and Silicon Is Bond-Centered Interstitial Muonium," T. L. Estle, S. Estreicher, and D. S. Marynick, *Hyperfine Inter*., **32**, 637-639 (1986).

74. "Localized Molecular Orbitals and Electronic Structure of Buckminsterfullerene," D. S. Marynick and S. Estreicher, *Chem. Phys. Lett.*, **132**, 383-385 (1986).

75. "Reply to a Comment on our Paper 'Surface Effects in Cluster Calculations ...,'" S. Estreicher, A. K. Ray, J. L. Fry, and D. S. Marynick, *Phys. Rev. Lett.*, **57**, 3301 (1986).

76. "The Electronic Structure of the Ditelluromercurate(II)Zintl Anion: A Scattered Wave X-α Study," F. U. Axe and D. S. Marynick, *Inorg. Chem.*, **26**, 1658-1664, (1987).

77. "A Molecular Orbital Study of Methyl Migration in Pentacarbonyl(methyl)manganese(I)," F. U. Axe and D. S. Marynick, *Organometallics*, **6**, 572-580 (1987).

78. "Bond-Centered Interstitial Hydrogen or Muonium in Diamond. The Explanation for Anomalous Muonium and an Example of Interstitial Metastability," T. L. Estle, S. Estreicher, and D. S. Marynick, *Phys. Rev. Lett.*, **58**, 1547-1550 (1987).

79. "Energetics of the Reaction Mn(H)(CO)‘Mn(HCO) Near the Hartree-Fock Limit," F. U. Axe and D. S. Marynick, *Chem. Phys. Lett.*, **141**, 455-458 (1987).

80. "Geometry, Optical and Magnetic Properties of $Cu(CO)_3$. A Theoretical Study," R. Arratia-Perez, F. U. Axe, and D. S. Marynick. *J. Phys. Chem.*, **21**, 5277-5283 (1987).

81. "Molecular Hyperfine Interactions in $Ag(CO)_3$," R. Arratia-Perez and D. S. Marynick, *J. Chem. Phys.*, **87**, 4644-4650 (1987).

82. "Ligand Exchange in η^5-Cyclopentadienyl(nickel)ligand Systems. A Theoretical Study," L. Throckmorton and D. S. Marynick, *J. Phys. Chem.,* **92**, 645-650 (1988).

83. "Electrochemical Synthesis and Optical Analysis of Poly[(2,2'-dithienyl)-5,5'-diylvinylene]," M. Martinez, J. R. Reynolds, S. Basak, D. A. Black, D. S. Marynick and M. Pomerantz, *Poly. Sci. Phys. Ed.,* **26**, 911-920 (1988).

84. "The Chemical Origins of Substituent Effects in Alkylpentacarbonylmanganese(I) Group Migration Reactions," F. U. Axe and D. S. Marynick, *J. Am. Chem. Soc.,* **110**, 3728-3734 (1988).

85. "Relationship Between Bonding and Structure in Tetranuclear Heteroatomic Zintl Anions Containing 20 Valence Electrons," F. U. Axe and D. S. Marynick, *Inorg. Chem.,* **27**, 1426-1431 (1988).

86. "Computational Evidence for an Unusual Transition State in the Fluxional Behavior of the Cyclopentadienyl Ligand in Chlorotris(cyclopentadienyl)titanium(IV)," L. M. Hansen and D. S. Marynick, *J. Am. Chem. Soc.,* **110**, 2358-2361 (1988).

87. "Paramagnetic Resonance Hyperfine Structure of Hexachloro Protactinate(IV)," R. Arratia-Perez and D. S. Marynick, *Phys. Rev. B.,* **37**, 4893-4899 (1988).

88. "Localized Molecular Orbitals of Simple Metal-Olefin Complexes," D. S. Marynick and C. M. Kirkpatrick, *J. Mol. Struct. THEOCHEM*, **169**, 245-256 (1988).

89. "Extended Basis Sets for Sc Through Zn," L. M. Hansen and D. S. Marynick, *J. Phys. Chem.,* **92**, 4588-4590 (1988).

90. "Electronic Structure Calculations on Large Organometallic Systems," Proceedings of the Cray Research, Inc. Second International Symposium, "Computational Chemistry on Cray Supercomputers," Chicago, Ill., Sept. 1988.

91. "Potential Energy Surface in Real Organometallic Systems," D. S. Marynick, F. U. Axe, L. Hansen and C. A. Jolly, *Topics in Physical Organometallic Chemistry*, Vol. 3, M. Gielen, ed., Freund Publishing, Israel, 1989, p. 37-74.

92. "Soluble Ethylmercapto Substituted Polythiophenes," J. P. Ruiz, J. R. Reynolds, K. Nayak, and D. S. Marynick, *Macromolecules*, **22**, 1231-1238 (1989).

93. "NMR Spectra of Heterocycles. Analysis of Carbon-13 Spectra of Thioxanthones Using Calculated Chemical Shifts, Substituent Constants, and PRDDO Molecular Orbital Calculations," J. S. Harwood, D. S. Marynick, and A. L. Ternay, Jr., *J. Chem. Soc. Perkins Tran. II*, 325-330 (1989).

94. "Hydrogen Passivation of Shallow Acceptors and Donors in C-Si: Comparisons and Trends," S. K. Estreicher, L. Throckmorton, and D. S. Marynick, *Phys. Rev. B*., **39**, 13241-13251 (1989).

95. "A Theoretical Study of the Direct Insertion Mechanism in a Real Ziegler-Natta Initiator: $Cp_2TiCH_3^+ + C_2H_4 \rightarrow Cp_2TiCH_2CH_2CH_3^+$," C. A. Jolly and D. S. Marynick, *J. Am. Chem. Soc.*, **111**, 7968-7974 (1989).

96. "Ground State Geometries and Inversion Barriers for Simple Complexes of Early Transition Metals," C. A. Jolly and D. S. Marynick, *Inorg. Chem.* **28**, 2893-2895 (1989).

97. "A Molecular Orbital Study of Conformational Preferences of the Cyclopentadienyl Ligand in Titanium(IV) and Titanium(III) Complexes," L. M. Hansen and D. S. Marynick, *Organometallics* **8**, 2173-2179 (1989).

98. "Equilibrium Structures of Neutral Interstitial Hydrogen in Zincblende BN and BP," S. K. Estreicher and D. S. Marynick, *Phys. Rev. B* **40**, 5739-5744 (1989).

99. "Synthesis, Characterization, Theoretical Modeling and Polymerization of New Fluorophore-Containing Derivatives of Thiophene and Pyrrole," S. Basak, K. Nayak, D. S. Marynick and K. Rajeshwar, *Chemistry of Materials* **1**, 611-619 (1989).

100. "Conformational and Intramolecular Hydrogen Bonding Effects on Post-emergence and Pre-emergence Selectivities of Herbicidal Pyrrole Dicarboxylates," T. A. Andrea, D. D. Stranz, A. Yang, D. A. Kleier, J. E. Powell, K. M. Patel, T. D. Price and D. S. Marynick, *Pestic. Sci.* **28**, 49-68 (1990).

101. "The Interplay between the Geometric and Electronic Structures of Polyisothianaphthene Polyisonaphthothiophen, Polythieno(3,4-6)pyrazine and Poly(3,4-6)quinoxaline," K. Nayak and D. S. Marynick, *Macromolecules* **23**, 2237-2245 (1990).

102. "Extended Slater Basis Sets for the Transition Metals Yttrium through Cadmium," L. Hansen and D. S. Marynick, *J. Comput. Chem.* **11**, 518-523 (1990).

103. "A Theoretical Study of Intramolecular Cis-Trans Isomerization Mechanisms in $Cr(CO)_5X$ (X = CO, PH_3 and PPh_3)," L. M. Hansen and D. S. Marynick, *Inorg. Chem.*, **29**, 2482-2486 (1990).

104. "Calculated Inversion Barriers and Proton Affinities of $P(CH_3)_3$ and $P(C_6H_5)_3$," C. A. Jolly, F. Chan, and D. S. Marynick, *Chem. Phys. Lett.*, **174**, 320-324 (1990).

105. "Computational Evidence for a Nonplanar η^3-Cyclopentadienyl Ligand in Dicarbonylbis-(cyclopentadienyl)chromium and the Pathway for the $\eta^5 \leftrightarrow \eta^3$ Ring Interchange," M. Lawless and D. S. Marynick, *Organometallics,* **10**, 543-545 (1991)

106. "Potential Energy Surfaces for Ring Inversion in Cp_2TiS_5," M. Lawless and D. S. Marynick, *Inorg. Chem.,* **30**, 3547-3551 (1991).

107. "Electrically Conducting Polymers Containing Alternating Substituted Phenylenes and Bithiophene Repeat Units," J. R. Reynolds, J. P. Ruiz, A. D. Child, K. Nayak, and D. S. Marynick, *Macromolecules*, **24**, 678-687 (1991).

108. "The Potential Energy Surfaces for Methyl Migration in Tetracarbonyl(methyl)cobalt(I) and Dicarbonylcyclopentadienyl(methyl)iron(II)," J. R. Rogers, O. Kwon and D. S. Marynick, *Organometallics*, **10**, 2817-2823 (1991).

109. "Potential Energy Surfaces for Ring Rearrangement Processes in Tricarbonyl(cyclo-octatetraene) chromium(0)," M. Lawless and D. S. Marynick, *J. Am. Chem. Soc.*, **113**, 7513-7521 (1991).

110. "Electrically Conduction Polymers Containing Substituted Phenylene and Heterocycle Repeat Units," J. P. Ruiz, A. D. Child, K. Nayak, D. S. Marynick, and J. R. Reynolds, *Synthetic Metals*, **41**, 783-788 (1991).

111. "Electronic Structure of the Polyatomic Zintl Anion Sb_7^{3-}, A Scattered-Wave Xα Study," C. A. Jolly and D. S. Marynick, *J. Mol. Struct. THEOCHEM.*, **253**, 9-16 (1992).

112. "Modified Extended Hückel Band Calculations on Conjugated Polymers," S. Y. Hong and D. S. Marynick, *J. Chem. Phys.*, **96**, 5497-5504 (1992).

113. "A Theoretical Study of the Conformations and Electronic Structures of Phenylene-pyrrole and Phenylene-furan Copolymers," S. Y. Hong and D. S. Marynick, *Macromolecules*, **25**, 3591-3595 (1992).

114. "Titanium and Copper in Si: Barriers for Diffusion and Interactions with Hydrogen," D. E. Woon, D. S. Marynick and S. K. Estreicher, *Phys. Rev. B*, **45**, 13,383-13,389 (1992).

115. "Understanding the Conformational Stability and Electronic Structure of Modified Polymers Based on Polythiophene," S. Y. Hong and D. S. Marynick, *Macromolecules*, **25**, 4652-4657 (1992).

116. "Ab initio Comparison of the Bonding Modes of Nitrate and Bicarbonate in Model Carbonic Anhydrase Systems," P. N. V. Pavan Kumar and D. S. Marynick, *Inorg. Chem.*, **32**, 1857-1859 (1993).

117. "Theoretical Estimates of the η^6 Bonding Capability of Buckminsterfullerene in Transition Metal Complexes," J. R. Rogers and D. S. Marynick, *Chem. Phys. Lett.*, **205**, 197-199 (1993).

118. "Substituent Effects on the Electrical Conductivity and Electrochemical Properties of Conjugated Furanyl Phenylene Polymers," J. R. Reynolds, A. D. Child, J. P. Ruiz, S. Y. Hong, and D. S. Marynick, *Macromolecules*, **26**, 2095-2103 (1993).

119. "Electronic Structure of the Coenzyme Vitamin B_{12} and Related Systems I. $Co(DH)_2(L)(R)$ Compounds (DH = Dimethylglyoxime; L = NH_3, py, 2-NH_2py, 5,6-Dimethylbenzimidazole; R = CH_3, i-C_3H_7, 5'-Deoxyadenosyl) as Model Systems for the Vitamin B_{12} Coenzyme," L. Hansen, P. N. V. Pavan Kumar, and D. S. Marynick, *Inorg. Chem.*, **33**, 728-735 (1994).

120. "Synthesis and Study of a Sulfur Heterocycle Fused *p*-Phenylene Vinylene Conducting Polymer. M. Pomerantz, J. Wang, S. Seong, K. P. Starkey, L. Nguyen and D. S. Marynick, *Phosphorus, Sulfur Silicon Relat. Elem.* **95 & 96**,506-508 (1994).

121. "Metal-Assisted Pyramidal Inversion in Metal-Phosphido Complexes," J. R. Rogers, T. P. S. Wagner, and D. S. Marynick, *Inorg. Chem.*, **33**, 3104-3110 (1994).

122. "Conformational Flexibility in C_2X_4-Bridged Bimetallic Complexes," J. R. Rogers, C. K. Johnson, and D. S. Marynick, *Inorg. Chem*., **33**, 4566-4572 (1994).

123. "The Performance of a Variety of Density Functional and Ab Initio Methods on the Structural Problem of Beryllium Borohydride," A. Derecskei-Kovacs and D. S. Marynick, *Chem. Phys. Lett.*, **228**, 252-258 (1994).

124. "Conformational Analysis of Tetrathiafulvalene Isomers and the Band Structure of Their One Dimensional Polymers," S. Seong and D. S. Marynick, *J. Phys. Chem.*, **98**, 13334-13338 (1994).

125. "Attachment of Two Electrons to $C_{60}F_{48}$: Coulomb Barriers in Doubly Charged Atoms," C. Jin, R. L. Hettich, R. N. Compton, A. Tuinman, A. Derecskei-Kovacs, D. S. Marynick, and B. I. Dunlap, *Phys. Rev. Lett.*, **73**, 2821-2825 (1994).

126. "Quantum Chemical Study of Boron Fullerene Analogs," A. Derecskei-Kovacs, B. Dunlap, W. N. Lipscomb, A. Lowrey, D. S. Marynick, and L. Massa, *Inorg. Chem.*, **33**, 5617-5619 (1994).

127. "Poly(benzo[1,2-*b*:4,5-*b*']dithiophene-4,8-diyl vinylene). Synthesis, Properties, and Electronic Structure of a New Dithiophene Fused *p*-Phenylene Vinylene Conducting Polymer," M. Pomerantz, J. Wang, S. Seong, K. P. Starkey, L. Nguyen, and D. S. Marynick, *Macromolecules*, **27**, 7478-7485 (1994).

128. "Potentially Stable Carbenes. A Theoretical Study of the Singlet-Triplet Separations, Proton Affinities, and Relative Metal Ion Affinities of Pyrazol-3-ylidene and Pyrazol-4-ylidene," L. L. Wall, R. Dias, and D. S. Marynick, *J. Molec. Struct. THEOCHEM*, **342**, 115-119(1995).

129. "Conformations and Electronic Structures of New Conjugated Polymers Based on Poly(cyclo-pentadienylene) and Polysilole," S. Y. Hong and D. S. Marynick, *Macromolecules*, 28, 4991-4995 (1995).

130. "Effects of Bridging Groups of Electronic Structures of Conjugated Cyclic Polymers," S. Y. Hong, S. J. Kwon, S.C. Kim and D.S. Marynick, *Synth. Met.,* **69**, 701-702(1995).

131. "Non-Empirical Wavefunctions for Very Large Molecules. I. The PRDDO/M Method," A. Derecskei-Kovacs and D. S. Marynick, *Internat. J. Quantum Chem.*, **58**, 193-202(1996).

132. "C_3Li_4 Revisited," D. S. Marynick and C. Hawkins, *Organometallics*, 15, 882-883(1996).

133. "Electronic Effects of Trifluoromethylated Tris(pyrazolyl)borate Ligands," H. V. Rasika Dias, H-J. Kim, H. L. Lu, A. Derecskei-Kovacs, N. Tacconi, K. Rajeshwar, and D. S. Marynick, *Organometallics*, **15**, 2994-3003(1996).

134. "Non-empirical Wavefunction for Very Large Molecules. II. Frozen Core Potentials within the PRDDO/M Approximations," A. Derecskei-Kovacs and D. S. Marynick, *Internat. J. Quantum Chem.*, **61**, 67-76(1997).

135. "Non-Empirical Wavefunctions for Very Large Molecules III. Extension of the PRDDO/M and PRDDO/M/FCP Methods to Main Row Elements Ga-Br," A. Derecskei-Kovacs and D. S. Marynick, *Internat. J. Quantum Chem.*, **63**, 1091-1097(1997).

136. "Noble-Gas-Related Defects in Si and the Origin of the 1018 meV Photoluminescence Line," S. K. Estreicher, J. Weber, A. Derecskei-Kovacs and D. S. Marynick, *Phys. Rev. B*, **55**, 5037-5044 (1997).

137. "Accurate Molecular Electrostatic Potentials Based on Modified PRDDO/M Wavefunctions. Part I: Electrostatic Potential Derived Atomic Charges," D. S. Marynick, *J. Comput. Chem*., **18**, 955-969(1997).

138. "Accurate Molecular Electrostatic Potentials Based on Modified PRDDO/M Wavefunctions. Part II: Electrostatic Potentials Inside the Molecular van der Waals Envelope," D. S. Marynick, *J. Comput. Chem*., **18**, 1682-1693(1997).

139. "Electronic Structure of Coenzyme B_{12} and Related Derivatives II. A Corrin Model System," L. M. Hansen, A. Derecskei-Kovacs and D. S. Marynick, *J. Mol. Struct. THEOCHEM*, **431**, 53-57 (1998).

140. "Conformational Preferences of 1, 3-diferrocenyl-1,1,3,3-tetramethyldisiloxane and Its Co-crystal with Ferrocene: A Theoretical and Crystallographic Study of the Role of Intra-and Intermolecular Interactions," F. Cervantes-Lee, H. Sharma, K. H. Pannell, A. Derecskei-Kovacs and D. S. Marynick, *Organometallics*, **17**, 3701-3706 (1998).

141. "PRDDO", D. S. Marynick, in "The Encyclopedia of Computational Chemistry," Schleyer, P. v. R.; Allinger, N. L., Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.; Schreiner, P. R. (Eds.); John Wiley & Sons: Chichester, 1998, vol. 2, pp. 1307-1313.

142. "Accurate Molecular Electrostatic Potentials Based on Modified PRDDO/M Wavefunctions. Part III: Parametrized Electrostatic Potential (PESP) Parameters for Li^+, Na^+, Mg^{2+}, K^+, Ca^{2+}, Zn^{2+} and I," D. S. Marynick, *J. Comput. Chem*., **18**, 1456-1469 (1998).

143. "The Application of Density Functional Theory to Four Problems in Inorganic Chemistry: A Comparison to Traditional ab Initio Methods," L. Wall, S. Wheeler, G. Wagenseller, and D. S. Marynick, *Inorg. Chem*, **37**, 3099-3106 (1998).

144. "Computational Estimates of the Gas-Phase Basicity and Proton Affinity of Glutamic Acid," W. Sun, G. R. Kinsel and D. S. Marynick, *J. Phys. Chem. A,* **103**, 4113-4117 (1999).

145. "A New Look at an Old Reaction: The Potential Energy Surface for the Thermal Carbonylation of $Mn(CO)_5CH_3$. The Role of Two Energetically Competitive Intermediates on the

Reaction Surface, and Comments on the Photo Decarbonylation of $Mn(CO)_5(COCH_3)$," A. Derecskei-Kovacs and D. S. Marynick, *J. Am. Chem. Soc*., **122**, 2078-2086 (2000).

146. "A Theoretical Study of the Molecular and Electronic Structures of Neutral Silver Bromide Clusters $(AgBr)_n$, n = 1, 9," H. Zhang, Z. A. Schelly and D. S. Marynick, *J. Phys. Chem.,* **104**, 6287-6294 (2000).

147. "Conformational Preferences of C_2X_4-Bridged Bimetallic Transition Metal Complexes," L. W. Mire and D. S. Marynick, *Inorg. Chem*, **39**, 5970-5975 (2000).

148. "Azido Derivatives of Low Valent Group 14 Elements: Synthesis and Characterization of [(*n*-Pr)$_2$ATI]GeN_3 and [(*n*-Pr)$_2$ATI]SnN_3 Featuring Heterobicyclic 10-π-Electron Ring Systems," A E. Ayers, D. S. Marynick and H. V. R. Dias, *Inorg. Chem.*, 39, 4147-4151 (2000).

149. "Copper and Silver Complexes Containing Organic Azide Ligands: Syntheses, Structures, and Theoretical Investigation of [HB(3,5-$(CF_3)_2Pz)_3$CuNNN(1-Ad) and [HB(3,5-$(CF_3)_2Pz)_3$AgN(1-Ad)NN (where Pz = pyrazolyl, and 1_Ad = 1-adamantyl)," H. V. R. Dias, S. A. Polach, S.-K. Goh, E. F. Archibong and D. S. Marynick, *Inorg. Chem*., **39**, 3894-3901 (2000).

150. "The Ability of Fullerenes to Act as η^6 Ligands in Transition Metal Complexes. A Comparative PM3(tm)-Density Functional Theory Study," S. K. Goh and D. S. Marynick, *J. Comput. Chem.,* **22**, 1881-1886 (2001).

151. "Ionization Energy Reductions in Small 2,5-Dihdroxybenzoic Acid / Proline Clusters," G. R. Kinsel, R. Knochenmuss, P. Setz, C. M. Land, S-K Goh, E. F. Archibong, J. H. Hardesty and D. S. Marynick, *J. Mass. Spec.,* **37**, 1131-1140 (2002).

152. "A Comparative DFT-MP2 Study of the Creutz-Taube Ion and Related Systems," S. K. Goh, J. Hardesty and D. S. Marynick, *J. Molec. Struct. THEOCHEM*, 588, 223-226 (2002).

153 "Methyl Migration in $(CH_3)Co(CO)_4$: A Detailed Density Functional Study," S. K. Goh and D. S. Marynick, *Organometallics*, **21**, 2262-2267 (2002).

154. "Structure and electron detachment energies of Al_3P^- and $Al_3P_3^-$," E. F. Archibong, S. K. Goh and D. S. Marynick, *J. Phys. Chem*. *A*, **106**, 5932-5937 (2002).

155. "On the Structure and Electron Photodetachment Spectra of Ga_3P^- and Ga_3As^-," E. F. Archibong, A. St-Amant, S. K. Goh, and D. S. Marynick, *Chem. Phys. Lett*., **361**, 411-420 (2002).

156. "On the Electronic Structure of AlP_3 and AlP_3^-," E. F. Archibong and D. S. Marynick, *Chem. Phys. Lett*., **361**, 214-218 (2002).

157. "Computational Estimates of the Gas Phase Acidities of Dihydroxybenzoic Acid Radical Cations and their Corresponding Neutral Species," F. H. Yassin and D. S. Marynick, *J. Molec. Struct. THEOCHEM*, **629**, 223-235 (2003).

158. "A Computational Study of the Electron Detachment Energies of $Al_2As_2^-$ and $Al_3As_3^-$," E. F. Archibong and D. S. Marynick, *Molecular Physics*, **101**, 2785-2792 (2003)

159. "Electron Spin Resonance Studies of Substituent Effects. 6. Experimental and Theoretical Studies of Ortho and Substituent-Induced Cis-Trans Isomerization in 1-Phenyl-1,2-Proopanesemidiones." E. T. Strom, D. S. Marynick, and B. S. Snowden, Jr, *Arkivoc*, **xiii**, 178-185 (2003).

160. "Arginine/2,5-Dihydroxybenzoic Acid Clusters: An Experimental and Computational Study of the Gas Phase and Solid State Systems," G. R. Kinsel, Q. Zhao, J. Narayanasamy, F. H Yassin, H. V. R. Dias, B. Niesner, K. Prater, C. St. Marie, L. Ly and D. S. Marynick, *J. Phys. Chem. A.,* **108***,* 3153-3161 (2004)

161. "Density Functional Study of the Molecular Structure of Lead Sulfide Clusters $(PbS)_n$, n = 1-9, H. Zeng, Z. A. Schelly and D. S. Marynick, *J. Phys. Chem.* A., **109**, 1616-1620 (2005).

162. "Computational Estimates of the Gas-Phase Basicities and Proton Affinities of the Six Isomers of Dihydroxybenzoic Acid," F. A. Yassin and D. S. Marynick, *Molecular Physics*, **103**, 183-189 (2005).

163. "Equilibrium Conditions in Laser Desorbed Plumes: Thermodynamic Properties of α-Cyano-4-hydroxycinnamic Acid and Protonation of Amino Acids," G. R. Kinsel, D. Yao, F. H. Yassin and D. S. Marynick, *European Mass Spectrometry*, *Eur.* **12(6)**, 359-367 (2006)

164. "A Computational Study of Matrix-Peptide Interactions in MALDI Mass Spectrometry: The Interactions of 2,5- and 3,5-Dihydroxybenzoic Acid with the Tripeptide Valine–Proline-Leucine," F. H. Yassin and D. S. Marynick, *J. Phys. Chem. A,* **110**, 3820 -3825 (2006).

165. "A Computational Study of the Thermodynamic Properties of Sinapic and Ferulic Acids and their Corresponding Radical Cations," F. H. Yassin and D. S. Marynick, *J. Molec. Struct. THEOCHEM*, **766**, 137-141 (2006).

166. "Cluster Precursors of Uncapped CdS Quantum Dots via Electroporation of Synthetic Liposomes. Experiments and Theory," H. Zeng, R. R.Vanga, D. S. Marynick, and Z. A. Schelly, *J. Phys. Chem. B,* **112 (46)**, 14422-14426 (2008).

167. "Computational Studies of Gas-Phase Ca_3P_2 and Ca_6P_4," C. S. P. Gamage, K. Ueno-Noto, and D. S. Marynick, J. *Phys. Chem. A***, 113**, 9737–9740 (2009**).**

168. "A Comparative Computational Study of Matrix-Peptide Interactions in MALDI Mass Spectrometry: The Interaction of Four Tripeptides with the MALDI Matrices 2,5-Dihyroxybenzoic Acid, alpha-Cyano-4-Hydroxy-Cinnamic Acid and 3,5-Dihyroxybenzoic Acid", K. Ueno-Noto and D. S. Marynick, *Molecular Physics*, **107**, 777-788 (2009).

COURSES TAUGHT

Chem 1284 Freshman Chemistry Laboratory

Chem 1301/1302	Freshman Chemistry
Chem 1301H/1302H	Honors Freshman Chemistry
Chem 2180, 4380	Undergraduate Research
Chem 3301	Introduction to Physical Chemistry
Chem 3321	Undergraduate Physical Chemistry I
Chem 3322	Undergraduate Physical Chemistry II
Chem 4331/5338	Group Theory
Chem 4391	Undergraduate Readings
Chem 5101	Graduate Seminar
Chem 5180	Quantum Chemistry Laboratory
Chem 5301	Graduate Physical Chemistry
Chem 5303	Graduate Physical Chemistry
Chem 4101	Senior Seminar
Chem 5315	Graduate Inorganic Chemistry
Chem 5334	Quantum Chemistry
Chem 6101	Topics in Graduate Research
Chem 6102	Issues in Modern Chemical Research

COMMITTEES

Department

Organized Research Fund Committee .....1979, 1983-1984 (chair)
Graduate Recruitment Committee ……1993-2001 (chair), 2002-2007
Undergraduate Curriculum Committee .....1979-82 (chair), 1984-1986
Graduate Advisor …… 1982-1986
New Faculty Selection Committees 1985-1987, 1989, 1991, 1993, 2005
Chairman Review Committee 1989
Chairman Selection Committee 1982-1983
Stockroom Committee 2002-2004
Committee on Graduate Studies .....1980-1989, 1990-2003(chair), 2003-2007
Promotion and Tenure Committee .....1979-81, 1983, 1986, 1988, 1990-1993, 1995-2001(chair), 2002-2007

College

Committee on Mathematical Sciences 1989-2007
Grade Appeals Committee 1997-2007
Undergraduate Curriculum Committee 1979-1982
Tenure and Promotions Committee……1989-1991
Organized Research Fund Committee .....1983 (chair), 1984
Research Enhancement Program Committee……. 1999, 2002

University

Research Integrity Committee…….2004-2007 (chair)
High Performance Computing Committee……..1998-2007 (chair)

Program Review Committee……2004-2007
Undergraduate Assembly…….2003-2007
Annual Celebration of Excellence by Students (ACES)
Organizing Committee…….……2003-2007
Information/Technology Compliance Subcommittee …….2000-2005
Academic Standards Committee 2000-2002
Teacher Education Council……..2002
Information/Technology Security Search Committee…….2002
Computing Facilities Committee .....1979-1988, 1989-1994 (chair)
Ad Hoc Computing Facilities Committee .....1983-1985 (chair)
Computing Planning Committee .....1989-1990 (chair)
Graduate Assembly 1982
Ad Hoc PC/Workstation Committee 1991-1993
Provost Advisory Council 1994-1995
SACS Computer Resources Committee 1996-1997

State/National
Lead scientific advisor for the NOVA episode "Linus Pauling: Crusading Scientist",
WGBH TV, Cambridge, MA.....1975
American Chemical Society Task Force on a Possible
Journal in the Field of Molecular Modeling 1992-1993
Center for High Performance Computing
User Advisory Committee (U. T. System).....1986-1989
American Chemical Society Examinations Committee
(Physical Chemistry Subcommittee).....1984-1986

BOOKS

Chemistry 1284 Laboratory Manual, a laboratory manual for first-year chemistry published "in house," September 1981.

HOBBIES

- Gourmet cooking, including contemporary Southwest, French, Chinese, Italian, BBQ and almost any other ethnic cuisine.
- Restaurant reviewing. I have written over 300 online restaurant reviews on various sites.
- Music, especially jazz, with an emphasis on bebop and other styles popular in the 40's-70's.
- Woodworking, including high-end furniture, restorations and everyday utilitarian items.
- Science Fiction