John A.W. Harkless

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Professional Preparation:

National Institute of Standards and Technology (NIST), Spring 2001-Summer 2002, National Research Council (NRC) Postdoctoral Researcher. Postdoctoral advisor, Dr. Karl Irikura: "Benchmark *ab initio* basis set and quantum Monte Carlo techniques for difficult systems."

University of California, Berkeley, Chemistry Department, Fall 1995-Spring 2001. Ph.D. in Chemistry. Thesis advisor, Professor William A. Lester, Jr.: "Novel Applications and Development of the Quantum Monte Carlo Method."

Morehouse College, Summer 1990-Spring 1995. Summa cum laude, B. S. in Chemistry and Mathematics, Phi Beta Kappa.

Research Experience:

October 2011 – present: Technology-enabled science communication and chemical education. Ongoing efforts through YouTube (http://youtube.com/johnharkless) to provide instructional assistance in the mechanics of understanding topics in General and Physical Chemistry. The YouTube channel has an international reach with ongoing addition of content in areas beyond college-level instruction.

September 2010 – June 2011: Visiting Research Analyst (VRA), The CNA Corporation. As an analyst for CNA, performed scientific analysis on topics of interest to the US Navy in addition to developing a model for the role of water availability in electrical power production with a focus on emerging technologies, alternative fuels, and environmental impact. An additional duty of the VRA position was to provide observations on possible mechanisms to improve recruitment and retention of African Americans as Research Analysts.

August 2009 – May 2010: MLK Visiting Professor of Chemistry, Massachusetts Institute of Technology. Ongoing research in quantum Monte Carlo (QMC) application to systems of interest and collaborative work investigating the role of multireference representations in QMC and coupled cluster approaches.

August 2008 – December 2008: Visiting Associate Professor of Chemistry, Louisiana State University. Ongoing research in QMC application to extended systems of transition metal, charged, and electronically excited species.

August 2007 – present: Associate Professor of Chemistry, Howard University. Continuing research in QMC application to transition metal systems, charged species, organic radicals and electronically excited molecules.

June 2007 – August 2007: Visiting Faculty Mentor, University of Cincinnati NSF Research Experience for Undergraduates (REU). Collaborative research in computational

biochemistry using β-Gaussian methods for normal mode analysis of chaperonins, as these structures have the potential to function as biological nanomachines.

August 2002- July 2007: Assistant Professor of Chemistry, Howard University, and guest researcher, National Institute of Standards and Technology (NIST). Continuing research in QMC application to transition metal systems, charged species, organic radicals and electronically excited molecules.

February 2001- July 2002: National Research Council (NRC) Postdoctoral Research Associate, NIST. Research program includes the application of QMC methods to prediction of excited electronic states of molecules and electronic structure of transition metal clusters. Distribution of QMC codes and training in the use of the code was also a goal of the NRC/NIST appointment.

Fall 1995-January 2001: Graduate Student. Advisor, Professor William A. Lester, Jr. Research in QMC methods and their application. Projects include determination of stability of highly reactive radical species of importance in soot formation, and extension of methodological capabilities. Performing QMC calculations requires proficiency in use of various quantum chemistry codes, e.g. GAMESS, Gaussian '94, HONDO, in addition to internal code development and distribution. Duties also included orienting new graduate student and postdoctoral researchers to the group and campus, Unix system administration and maintenance, and developing networking and technology solutions for the group.

Summer 1995: AT&T Bell Labs Cooperative Research Fellowship summer intership. Mentor: Dr. Frank H. Stillinger. Silicon nanocrystal calculations. Developed and implemented codes written in FORTRAN for RS600 workstations, as well as used mathematical analysis codes (e.g., Mathematica, Theorist, Matlab, etc.)

Summer 1994: AT&T Bell Labs Summer Research Program. Mentor: Dr. Frank H. Stillinger. Structure and energy calculations for SiO_2 clusters. Developed and implemented codes written in FORTRAN for RS6000 workstations.

Summer 1994, '93, '92: NASA Kennedy Space Center. X-Ray fluorescence and Auger/X-Ray Photoelectron Spectroscopy. Work included use of proprietary automation languages in development of user-friendly interfaces for x-ray fluorescence equipment.

Summer 1991: NASA Stennis Space Center. Participated in a team that implemented chemical tracking and hazards database. Work involved cataloguing inventories and generating CAD layouts of buildings.

Instructional Experience:

Fall 2021, 2020, 2007: Instructor, Advanced Physical Chemistry I, Howard University. Graduate course that covers topics in thermodynamics and statistical mechanics. This course emphasized the connection between the mathematical representations of chemical systems and the physical relevance of conclusions that may be drawn from the models presented. Students were encouraged to learn to think of chemical systems at both micro- and macro-scale phenomena as described by thermodynamical and statistical processes.

Spring 2021, 2020: Instructor, Advanced Physical Chemistry II Lecture, Howard University. Graduate-level course with a focus on quantum mechanics, spectroscopy, and kinetics. Graduate students are instructed not only in the fundamentals and theory of these topics, but also how they integrate into the modern enterprise of chemical investigations and discovery.

Spring 2018, 2017, 2016, 2015: Instructor, General Chemistry I Laboratory, Howard University. Course introduces basic concepts in physical, inorganic, and analytical chemistry. Students develop the skills needed to generate, capture, and analyze data to be able to draw conclusions about the behavior and manipulation of chemical systems.

Spring 2021, 2020, 2018, 2017, 2016, 2015, 2014, 2013: Instructor, Physical Chemistry II, Howard University. Upper-division course that covers topics in in the principles and application of quantum mechanics with respect to atomic and molecular structure and spectroscopy, and kinetics with respect to prediction and control of reactions. This course represents a significant redesign in the sequencing and organization of topics to emphasize that quantum mechanics explains why spectroscopy works and the reasons why the modern chemist should know it. This iteration of the course successfully integrated the YouTube channel (http://youtube.com/johnharkless/) that provided supplemental instruction on the problem-solving philosophies used in physical chemistry.

Fall 2019, 2016, 2015, 2014: Instructor, Computational Methods in Chemistry, Howard University. Graduate course that covers the principle and practice of ab initio, and DFT computational techniques; successful completion implies a basic understanding of computational software and of the underlying methodologies. This course was complemented by a partnership with CLDC, a computational science laboratory in the College of Engineering, Computer and Architectural Sciences.

Fall 2021, 2020, 2019, 2017, 2016, 2015, 2014, 2013: Instructor, Physical Chemistry I, Howard University. Standard undergraduate course explaining the details of the origin of chemical measurement through a combination of statistical mechanics and thermodynamics. This course includes significant online components and a course structure designed to serve the needs of upper-level undergraduates in the chemical sciences and engineering. This iteration of the course successfully integrated the YouTube channel (http://youtube.com/johnharkless/) that provided supplemental instruction on the problem-solving philosophies used in physical chemistry. One key difference in this course is the inclusion of practical problem-solving and team-based exercises.

Spring 2013, 2012: Instructor, General Chemistry II, Howard University, a continuation of the first undergraduate course in chemistry. Topics included kinetics, equilibrium and non-equilibrium chemistry as related to solutions, electrochemistry, and acid-base

chemistry, in addition to a unit on nuclear chemistry. This version of the course completely integrated the YouTube channel (http://youtube.com/johnharkless/) and a stronger emphasis on problem-solving, synthesis of basic chemical understanding, and self-directed learning.

Fall 2012, 2011: Instructor, General Chemistry I, Howard University. Standard undergraduate course introducing students to basic concepts in chemistry, including atomic and molecular structure, basic thermodynamics, and gas laws. This course includes significant online components and a course structure designed to benefit students at all levels of preparation in the chemical sciences. This iteration of the course successfully capitalized on social media via @HUGenChem on Twitter, and integrated a YouTube channel (http://youtube.com/johnharkless/) that provided self-paced instruction on the mechanics of problem-solving in chemistry.

Fall 2012: Instructor, General Chemistry I Laboratory, Howard University. Course introduces basic concepts in physical, inorganic, and analytical chemistry. Students develop the skills needed to generate, capture, and analyze data to be able to draw conclusions about the behavior and manipulation of chemical systems.

Fall 2011: Instructor, General Chemistry I Laboratory, Howard University. Course introduces basic concepts in physical, inorganic, and analytical chemistry. Students develop the skills needed to generate, capture, and analyze data to be able to draw conclusions about the behavior and manipulation of chemical systems.

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Spring 2008: Instructor, Computational Methods in Chemistry, Howard University. Graduate course that covers the principle and practice of ab initio, and DFT computational techniques; successful completion implies a basic understanding of computational software and of the underlying methodologies. This course was complemented by a partnership with CLDC, a computational science laboratory in the College of Engineering, Computer and Architectural Sciences.

Spring 2008: Co-Instructor, Physical Organic Chemistry. Graduate course that covers topics in the underlying physical aspects of organic chemistry, with an emphasis on the principles that guide modern thought in organic chemistry. Instructional efforts in this course included development of modules to integrate theoretical and computational chemistry into the curriculum, including examples from Huckel theory, semi-empirical, and fully ab initio molecular orbital calculations.

Fall 2007: Instructor, Physical Chemistry Laboratory I, Howard University. This course was completely re-engineered to modernize the principles and practices communicated to

the students enrolled.Undergraduate laboratory course for chemistry majors. Experiments in this laboratory course demonstrate principles in thermodynamics and kinetics.

Fall 2007: Co-Instructor, Physical Chemistry II, Howard University. Undergraduate course in quantum mechanics and spectroscopy. This special section was team taught by three instructors, covering topics in kinetics, quantum mechanics, and spectroscopy. Instructional efforts in this course required development of a self-contained curriculum in quantum mechanics.

Spring 2007: Instructor, Computational Methods in Chemistry, Howard University. Graduate course that covers the principle and practice of computational modeling.

Fall 2006: Instructor, Advanced Physical Chemistry I, Howard University. Graduate course that covers topics in thermodynamics and kinetics.

Fall 2006: Instructor, Physical Chemistry Laboratory I, Howard University. Undergraduate laboratory course for chemistry majors. Experiments in this laboratory course demonstrate principles in thermodynamics and kinetics.

Spring 2006: Instructor, Computational Methods in Chemistry, Howard University. Graduate course that covers the principle and practice of computational modeling.

Fall 2005: Instructor, Advanced Physical Chemistry I, Howard University. Graduate course that covers topics in thermodynamics and kinetics.

Fall 2005: Instructor, Physical Chemistry Laboratory I, Howard University. Undergraduate laboratory course for chemistry majors. Experiments in this laboratory course demonstrate principles in thermodynamics and kinetics. This course was completely re-engineered to modernize the principles and practices communicated to the students enrolled.

Spring 2005: Instructor, Computational Methods in Chemistry, Howard University. Graduate course that covers the principle and practice of computational modeling.

Spring 2005: Instructor, General Chemistry II, Howard University, a continuation of the first undergraduate course in chemistry. Topics included kinetics, equilibrium and non-equilibrium chemistry as related to solutions, electrochemistry, and acid-base chemistry, in addition to a unit on nuclear chemistry. This course includes significant online components and a course structure designed to benefit students at all levels of preparation in the chemical sciences.

Fall 2004: Instructor, General Chemistry, Howard University. Standard undergraduate course introducing students to basic concepts in chemistry, including atomic and molecular structure, basic thermodynamics, and gas laws. This course includes significant online components and a course structure designed to benefit students at all levels of preparation in the chemical sciences.

Spring 2004: Instructor, General Chemistry II, Howard University, a continuation of the first undergraduate course in chemistry. This course includes significant online components and a course structure designed to benefit students at all levels of preparation in the chemical sciences.

Fall 2003: Instructor, General Chemistry, Howard University. Standard undergraduate course introducing students to basic concepts in chemistry. This course includes significant online components and a course structure designed to benefit students at all levels of preparation in the chemical sciences.

Spring 2003: Instructor, Computational Methods in Chemistry, Howard University. Graduate course that covers the principle and practice of most computational techniques; successful completion implies a basic understanding of computational software and of the underlying methodologies. This course was complemented by a small grant of computer time from the San Diego Supercomputing Center.

Fall 2002: Instructor, Physical Chemistry II Lecture, Howard University. Second-semester undergraduate course covered topics in quantum mechanics and spectroscopy. This course contained significant writing assignments.

Fall 1997: Graduate Student Instructor, General Chemistry, College of Chemistry Scholars Program (CoCSP), UC Berkeley. Planned and lead intensive discussion and laboratory sections, designed to promote and advance the educational and career opportunities of students from traditionally disadvantaged and underrepresented backgrounds in the fields of chemistry and chemical engineering.

Summer 1996, 1997: MESA (Math, Engineering, Science Achievement) Program, University of California, Berkeley. Field trip director. Organized engineering and science field trips for MESA Junior High Summer Academy.

Fall 1996: Graduate Student Instructor, Quantitative Analysis, UC Berkeley. Performed teaching assistant functions in laboratory and lecture for the departmental service course in quantitative analysis.

Fall 1995: Graduate Student Instructor, General Chemistry Laboratory, UC Berkeley. Was responsible for two sections of laboratory, including pre-lab lectures and demonstrations.

Spring 1994-Spring 1995: Mathematics and Chemistry Tutor, Morehouse College. Paid and volunteer work tutoring students in lower division and select upper division courses.

Fall 1993-Fall 1994: Mathematics Teaching Assistant, Morehouse College Adult Education program. Duties included assisting lead instructor in teaching GED-level mathematics.

Grantsmanship:

Spring 2015: Research equipment grant, Co-PI. An internal research initiation grant, co-authored with a colleague in Mathematics. The purpose of the grant was to create an in-house resource for computational science within the College of Arts and Sciences at Howard University.

Fall 2012: NSF Partnership for Reduced-Dimensional Materials (PRDM), Participant. A Multi-institution, multi-researcher grant between Cornell, Howard, and Gallaudet Universities and Prince George's Community College to collaboratively model, design and fabricate materials at the molecular and nano scales with novel properties.

Spring 2006: Army High Performance Computing Research Center- AHPCRC (renewed). Annually renewable grant to support personnel performing research relevant

to the Army HPC Nanoscience Portfolio, and additional funding to support research and technology transfer between Howard University and other AHPCRC member institutions.

Spring 2005: Army High Performance Computing Research Center- AHPCRC (renewed). Annually renewable grant to support personnel performing research relevant to the Army HPC Nanoscience Portfolio, and additional funding to support research and technology transfer between Howard University and other AHPCRC member institutions.

Spring 2004: AHPCRC. Annually renewable grant to support personnel performing research relevant to the Army HPC Nanoscience Portfolio, and additional funding to support workshops in computational biophysics and drug design.

Fall 2003: NSF CREST Center for Nanomaterials Science and Characterization. Co-PI on the five-year award for center to design, fabricate, and characterize novel materials at the nanoscale.

Publications:

A. Gibson, J. Harkless, M. Alexander, and K.R. Scott, "Enaminones 10. Molecular Modeling Aspects of the 5-Methylcyclohexenone derivatives", Bioorganic and Medicinal Chemistry, **2009**, vol. 17, no. 14, pp 5342-5346. DOI:10.1016/j.bmc.2009.03.068

Collins, Sibrina N.; Holt, Herman L., Jr.; Harkless, John A.; Gudmundsdottir, Anna D.; Ault, Bruce S. "Visiting Faculty Mentors as a Component of an NSF-REU Program", J. Chem. Educ. **2009,** vol. 86, p. 565.

F. A. Fayton, Jr., A. A. Gibson, and J. A. W. Harkless, "Prediction of excited state energies for molecular nitrogen using quantum Monte Carlo methods", International Journal of Quantum Chemistry **2008**, vol. 109, no. 1, pp 43-49.

J.A. W. Harkless and J. S. Francisco, "Bond Dissociation and Conformational Energetics of Tetrasulfur: A Quantum Monte Carlo Study" Journal of Physical Chemistry, January 25, **2008**, vol. 112, no. 10, pp 2098-2092.

M.H. Matus, D.A. Dixon, K. A. Peterson, J.A.W. Harkless, and J.S. Francisco, "Coupled-Cluster study of the electronic structure and energetics of tetrasulfur, S_4" Journal of Chemical Physics, November 5, **2007**, vol. 127, p 174305.

J. A. W. Harkless and K. K. Irikura, "Multi-determinant Trial Functions in the Determination of the Dissociation Energy of the Beryllium Dimer: a Quantum Monte Carlo Study" International Journal of Quantum Chemistry, April 24, **2006**, vol. 106, No. 11, pp 2373-2378.

J. A. W. Harkless, L. Mitas, J. R. Rodriguez, and W. A. Lester, Jr. "A Quantum Monte Carlo Study of the Electronic Structure of Peroxynitrite Anion." Journal of Chemical Physics, March 15, **2003**, vol. 118, No. 11, pp 4987-4992.

J. A. W. Harkless and W. A. Lester, Jr., "Quantum Monte Carlo for Atoms and Molecules, "Proceedings of the Workshop on Contemporary Problems in Mathematical Physics, World Scientific Publishing (Singapore), p. 153, **2000**.

J. A. W. Harkless and W. A. Lester, Jr. "Quantum Monte Carlo determination of the atomization energy and heat of formation of propargyl radical." Journal of Chemical Physics, August 15, **2000**, vol. 113, No. 7, pp. 2680-2683

L. E. Brus, J. A. W. Harkless, and F. H. Stillinger. "Theoretical Metastability of Semiconductor Crystallites in High-Pressure Phases, with Application to beta-Tin Structure Silicon." Journal of the American Chemical Society, **1996** May 22, vol. 118, No. 20, pp. 4834-4838.

J. A. W. Harkless, D. K. Stillinger, and F. H. Stillinger. "Structures and Energies of SiO_2 Clusters." Journal of Physical Chemistry, **1996** Jan. 25, vol. 100, No. 4, pp. 1098-1103.

J. A. W. Harkless. "New X-Ray Fluorescence (XRF) Programs." NASA Tech Briefs, 1996.

Presentations and Posters:

February 2020: Black Engineer of the Year Awards (BEYA) Leading Voices Event "Quantum: Concepts to Chemistry to Computing"

October 2019: Walter E. Massey Seminar Series, Morehouse College: "Solving the Chem-Mystery and Moving Beyond the Equations"

July 2021, 2020, 2019: NCAS-M ETSP Summer Program Workshop: "Choosing a Medium and Speaking On Camera"

June 2018: Capstone Institute, Workshop: "A Classroom Chemistry: Making Meaning Mean More"

April 2018: Howard University Tau Beta Pi Seminar: "Science U R Doin It Rong"

March 2018: Preparing Future Faculty Workshop: "Teaching With YouTube"

June 2017: Capstone Institute, Workshop: "Making Science Fun, or, Making Fun of Science?"

March 2017: Preparing Future Faculty Workshop: "Learning Through Play"

August 2016: Capstone Institute, Workshop: "Learning Through Play: Gamifying Science and Math Education"

June 2015: ACS Northeast Regional Meeting, Presentation: "Beyond Percy Julian: Howard University Chemical History As American Chemical History"

March 2015: University of California, San Diego, Presentation: "A Difference in Perspective: How Being a Minority Chemist Aids Chemical Intuition"

June 2014: Capstone STEM Summer Professional Development Institute, Workshop: "Storytelling in STEM: Creating Long-Form Narratives In the Classroom"

May 2014: University of Pennsylvania, NOBCChE chapter presentation: "The Research Life of a Minority Chemist: How a Difference in Perspective Aids Chemical Intuition"

August 2013: Capstone Summer Institute, Workshop on collaborative planning with Prezi

April 2013: 241st ACS Annual Meeting, Presentation: ""Electronic Structure of Sulfur-Containing Compounds"

March 2013: American Physical Society, Presentation: “A Perspective on the Intersection of Institutional Identity and Collaborative Research: Toward More Effective Partnering With Historically Black Colleges and Universities (HBCUs)”

September 2012: NOBCChE 39th Annual Conference, Presentation: “Electronic Structure of Sulfur-Containing Compounds”

March 2012: NOBCChE West Regional Meeting, Presentation: “Chemistry Beyond Chemicals”

April 2011: NOBCChE 37th Annual Conference, Presentation: “Electronic Structure Of Potentially Conductive Polymers: Relevant To Electrical Storage And Transmission?”

December 2010: Pacifichem, Presentation: “Procedural wavefunctions for difficult systems: quality with less complexity?”

October 2010: Nigerian Society of Chemical Engineers, Presentation: “Electronic Structure Of Potentially Conductive Polymers: Relevant To Electrical Storage And Transmission?”

March 2010: 235th ACS Annual Meeting, Presentation: “Estimates of S_n (n=1-4) electronic excited state energies”

March 2010: 235th ACS Annual Meeting, Presentation: “HBCU partnerships and pedigrees: The interaction of institutional and personal identity”

March 2010: NOBCChE 36th Annual Conference, Workshop: "Earning Tenure"

March 2010: NOBCChE 36th Annual Conference, Presentation: "Electronic Structure of Sulfur Compounds: Bonding and Excited States"

November 2009: Jackson State University, Presentation: “Quantum Mechanics and Chemical Intuition, or ‘Where Did That Electron Go?’”

September 2009: NOBCChE Northeast Regional Meeting, Presentation: “Simplified Quantum Monte Carlo Trial Function Design for “Difficult” Systems”

March 2009: NOBCChE 35th Annual Conference, Presentation: “High-Accuracy ab initio Studies of S_n (n=1-4) Electronic Structure”

November 2008: Xavier University of Louisiana, Presentation: “Quantum Mechanics and Chemical Intuition, or ‘Where Did That Electron Go?’”

August 2008: 234th ACS Annual Meeting, Presentation: “High-accuracy ab initio studies of tetrasulfur energetics”

July 2008: 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Presentation: “Simplified QMC Trial Function Design for ‘Difficult’ Systems”

March 2008: NOBCChE 34th Annual Conference, Presentation: “High-Accuracy ab initio studies of S_4 energetics”

April 2007: William A. Lester, Jr. Symposium, Presentation: “High-Accuracy ab initio studies of S_4 energetics”

March 2006: 231st ACS Annual Meeting, Presentation: “High-Accuracy ab initio studies of S4 conformer energetics”

August 2005: 230th ACS Annual Meeting, Presentation: “Quantum Monte Carlo estimation of properties of novel nanoscale compounds.”

August 2005: 230th ACS Annual Meeting, Presentation: “Electronic structure of ‘difficult’ systems: Quantum Monte Carlo estimates of transition metal IP and EA.”

August 2005: 230th ACS Annual Meeting, Poster: “Electronic Structure Theory for Nanomaterials Science: Quantum Monte Carlo for ‘Difficult’ Systems.”

August 2004: 228th ACS Annual Meeting, Poster: “Performance of post-Hartree Fock, density functional theory, and quantum Monte Carlo methods for the electronic structure of 3d-block transition metals.”

August 2004: 228th ACS Annual Meeting, Poster: “Electronic structure research: Quantum Monte Carlo, traditional *ab initio*, and density functional approaches in the study of ‘difficult’ chemical systems.”

August 2004: 228th ACS Annual Meeting, Presentation: “Personal narrative on training at a majority and teaching at a minority research institution.”

April 2004: NOBCChE 30th Annual Conference, Presentation: “Multi-Determinant Trial Functions in the Determination of the Dissociation Energy of the Beryllium Dimer: a Quantum Monte Carlo Study.”

November 2003: 12th Conference on Current Trends in Computational Chemistry, Poster: “Multi-determinant Trial Functions in the Determination of the Dissociation Energy of the Beryllium Dimer: a Quantum Monte Carlo Study.”

March 2002: NOBBChE 28th Annual Conference, Presentation: “A Quantum Monte Carlo Study of the Excited States of Ozone.”

February 2002: NIST Sigma Xi Poster: “Quantum Monte Carlo Estimate of the Dissociation Energy of Beryllium Dimer”

November 2001: 10th International Conference on Current Trends in Computational Chemistry, Poster: "Quantum Monte Carlo Studies of the Ozone Molecule."

June 2001: 56th Ohio State University International Symposium On Molecular Spectroscopy, Presentation: "Comparative Excited State Studies of Selected Species Using Quantum Monte Carlo."

April 2001: NOBCChE 27th Annual Conference, Presentation: "Quantum Monte Carlo for Difficult Systems"

February 2001: NIST Sigma Xi Poster: "Quantum Monte Carlo for Difficult Systems"

January 2000: Pitzer 2000 Symposium, Poster: "Energy Gradients and Higher-Order Derivatives in Quantum Monte Carlo via Likelihood Ratios"

November 1999: 1st Workshop on Contemporary Problems in Mathematical Physics, Cotonou, Republic of Benin, Presentation: "Quantum Monte Carlo Study of the Propargyl Radical" and "Quantum Monte Carlo Applications for Molecular Systems"

April 1999: NOBCChE 26th Annual Conference, Presentation: "Energy Gradients and Higher-Order Derivatives in Quantum Monte Carlo via Likelihood Ratios"

March 1999: American Chemical Society Spring Meeting, Poster: "Energy Gradients and Higher-Order Derivatives in Quantum Monte Carlo via Likelihood Ratios"

November 1998: 7th Conference on Current Trends in Computational Chemistry, Poster "Energy Gradients in Quantum Monte Carlo via Likelihood Ratios"

October 1998: National Society of Black Engineers (NSBE) Region 6 Fall Conference, Presentation: "Effective Time Management Strategies for Students"

August 1998: Bell Labs Cooperative Research Fellows Program Poster Session, Poster: "Quantum Monte Carlo Study of the Propargyl Radical and Other Hydrocarbon Systems"

June 1998: 53rd Ohio State University International Symposium On Molecular Spectroscopy, Presentation: "Ground-State Properties of the Propargyl (C_3H_3) Radical: A Quantum Monte Carlo Study"

November 1997: 6th Conference on Current Trends in Computational Chemistry, Poster: "Quantum Monte Carlo Study of the Propargyl Radical"

Fellowships, Honor Societies, Awards and Organizations:

- Massachusetts Institute of Technology Martin Luther King visiting Professor of Chemistry, 2009-2010
- Henry C. McBay Outstanding Teacher Award, NOBCChE, 2007
- NIST/NRC Postdoctoral Researcher, 2001-2002
- Phi Beta Kappa National Honor Society, inducted 1993
- Bell Labs Cooperative Research Fellowship, 1995-2000
- Chancellor's Graduate Opportunity Fellowship, UC Berkeley, 1995-2001
- American Chemical Society Division of Physical Chemistry/ IBM Graduate Student Award in Computational Chemistry, second place, 1998
- Eastman Kodak Dr. Theophilus Sorrell Award, NOBCChE, 1999
- Black Graduate Engineering and Science Students (BGESS), President 1997-1998. Led fundraising, gaining funds in excess of $10,000. Co-coordinated BGESS 1998 Science Fair, in conjunction with UC Berkeley Electrical Engineering and Computer Science Department, for students from two high schools in Oakland. Inaugurated a speaker series funded by LAM Research.
- BGESS Undergraduate Liaison, 1998-1999. Developed networking groups for African-American graduate and undergraduate students by major in engineering, mathematics and the sciences.
- Alpha Phi Alpha Fraternity, Inc. 2006-present.

Service Activities and Affiliations:

Phi Beta Kappa Society, Senator. As a member of the Board of Directors, I share responsibility for governance and promotion of the goals of the Society.

Phi Beta Kappa Society, member, Committee of Qualifications (CQ). CQ oversees the process of vetting applications for new chapters of Phi Beta Kappa to be sheltered at select institutions of higher learning.

American Chemical Society (ACS) Executive Director's 2020 Committee. Member of the committee selected to study and suggest developing an enhanced value proposition for the future of the ACS, with the expectation of increasing membership recruitment and retention.

Army HPCRC Workshop Organizer: "Frontiers in Computational Biophysics and Drug Design," to be hosted by Howard University, Oct. 21-22, 2004. First workshop sponsored by the Army HPCRC to bring together researchers inside and outside of the Army HPC research community to discuss topics in protein structure prediction, computational drug design and computational biophysics.

National Science Foundation Workshop, "Workshop on Cyber-Enabled Chemistry," October 3-5, 2004. The primary purpose of this workshop was to identify key issues in Cyber-Infrastructure that face the chemistry community, and to explore potential solutions to addressing these issues. The approximately 50 invited participants included representatives from academia, government and industry.

American Chemical Society (ACS) Executive Director's 2020 Committee. Member of the committee selected to study and suggest developing an enhanced value proposition for the future of the ACS, with the expectation of increasing membership recruitment and retention.

National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE), National Vice-President, 2007 – 2011, and National Technical Program Committee, Chair, 2003-2007. Chair of the committee in charge of organizing the technical program for the annual meeting of NOBCChE. Duties include management of volunteer staff and program scheduling.

Computing and Instrumentation Committee, Howard University Department of Chemistry. Chair, 2003-2004. Committee is in charge of assessing and developing the computational and instrumentation needs of the department, and has developed a schedule of user fees for internal and external use of major instrumentation.

Academic Advising Committee, Howard University Department of Chemistry. Lead advisor, 2002 – 2006. Responsible for revamping the advising of chemistry majors by faculty, leading to improved satisfaction of majors and increased efficiency of advising. Duties also include maintaining accurate, up-to-date information of academic policies as well as redevelopment and updating of course curriculum and graduation schemes.