

## Curriculum Vitae Dr. David A. Dixon

Robert Ramsay Chair  
Department of Chemistry  
The University of Alabama

### Birth Date

Dec. 3, 1949 in Houston, Texas

### Address

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### Education

B.S. with honors, Chemistry, California Institute of Technology, Pasadena, California, June 1971  
Ph.D., Physical Chemistry, Harvard University, Cambridge, Massachusetts, completed June 1975 (received March 1976)

Thesis Supervisors: Professors D.R. Herschbach and W.N. Lipscomb

Thesis Title: *I. Reactions of van der Waals Molecules. II. Localized Molecule Orbitals for Polyatomic Molecules*

### Positions Held

*Junior Fellow*, Society of Fellows, Harvard University, Cambridge, Massachusetts, 7/1975 - 6/1977.

*Visiting Associate*, Chemistry, California Institute of Technology, Pasadena, California, 2/1977 - 6/1977.

*Assistant Professor*, Chemistry Department, University of Minnesota, Minneapolis, Minnesota, 9/1977 - 6/1983.

*Member of Research Staff*, Chemical Sciences, Central Research and Development Department, E.I. du Pont de Nemours and Co., Inc. Wilmington, Delaware, 7/1983 - 9/1995

*Research Leader*, computational chemistry, Central Research and Development, E. I. du Pont de Nemours and Co., Inc., Wilmington, Delaware, 1990 - 9/1995.

*Research Fellow*, DuPont Central Science and Engineering Laboratories, Experimental Station, Wilmington, Delaware, 1992 - 9/1995

*Associate Director*, Theory, Modeling & Simulation, Environmental Molecular Science Laboratory, Pacific Northwest National Laboratory, 9/1995- 9/2002

*Battelle Fellow*, Pacific Northwest National Laboratory, 10/2002 – 12/2003

*Professor of Chemistry*, University of Alabama – Tuscaloosa, 1/2004 –

*Robert Ramsay Chair*, Department of Chemistry, University of Alabama – Tuscaloosa, April, 2004 –

*Interim Chair*, Department of Chemistry, University of Alabama – Tuscaloosa, Aug., 2007- Aug. 2008

*Joint appointment* – Argonne National Laboratory, 2010-

### **Awards**

1967, National Merit Scholarship (Honorary)

1967, California Institute of Technology Scholarship

1968-1971, ARCS Scholarship, Caltech

1970, Tau Beta Pi

1971, Green Award (for Undergraduate Research), Caltech

1974, Teaching Fellow Prize, Harvard University

1974, Parker Fellowship, Harvard University

1975, NATO Summer School Fellowship

1975 – 1977, Junior Fellow, Society of Fellows, Harvard University

1976, Class Marshall, Graduate School of Arts and Science, Harvard University

1977-1981, Alfred P. Sloan Research Fellowship

1978-1983, Camille and Henry Dreyfus Teacher-Scholar

1981, Sigma Xi

1982, Phi Kappa Phi

1982, George Taylor/I.T. Alumni Society Research Award, Inst. of Technology, University of Minnesota,

1989, Leo Hendrik Baekeland Award of the American Chemical Society

1994, Fellow-American Association for the Advancement of Science

2000, Federal Laboratory Consortium Technology Transfer Award

2002, Fellow of the American Physical Society, Division of Chemical Physics

2002, European Academy of Sciences

2003, American Chemical Society Award for Creative Work in Fluorine Chemistry

2006, Computer Based Honors Program, The University of Alabama, Outstanding Computer Based Honors Project Director

2007, 20<sup>th</sup> Charles A. Coulson Lecture, Department of Chemistry, University of Georgia

2010, DOE Hydrogen Program R&D Award for Outstanding Contributions to Hydrogen Storage Technologies

2011, Burnum Award, The University of Alabama

2012, The University of Alabama SEC Faculty Achievement Award (Inaugural Award)

2013, Fellow, American Chemical Society

2015, Distinguished Service Award, Division of Fluorine Chemistry, American Chemical Society

### **Teaching Experience**

1971-75, Teaching Fellow, Harvard University in General Chemistry, Physical Chemistry Laboratory, Molecular Orbital Theory

1977-83, Assistant Professor, University of Minnesota, General Chemistry, graduate and undergraduate Physical Chemistry and Quantum Chemistry, and graduate Theoretical Organic Chemistry, supervised 5 Ph.D. theses

1986, 2<sup>nd</sup> Semester Graduate Quantum Mechanics, Winter/Spring, University of Pennsylvania.

2004, 2005 (Fall), Introductory Chemistry II

2004-present, Computer Based Honors Program

2006 (Spring), Graduate Statistical Mechanics, Thermodynamics, and Kinetics

2006-2012 (Fall), Honors Introductory Chemistry I

2006, 2007, 2011, 2012, 2013, 2014 (Fall), Freshman Learning Community

2013-2015 (Fall) Physical Chemistry (Quantum Mechanics) for ACS undergraduate majors and chemistry graduate students

### **Adjunct Positions**

1986 Winter/Spring, Adjunct Faculty, Chemistry Department, University of Pennsylvania,.

1987 Spring, Adjunct Professor, Georgia Institute of Technology, Chemistry Department,

1/89 – 1999, Adjunct Professor, University of Delaware, Chemistry Department.

4/97 – 2003, Adjunct Professor, University of Utah, Chemistry Department

1997 Fall, Visiting Scholar at the Autonomous Metropolitan University, Mexico City, Celebration of the 20<sup>th</sup> anniversary of the Chemistry Department.

### **Selected External Committees and Workshops**

1987 Raveché Panel that wrote "A National Computing Initiative"

1988 Planning Committee: 2<sup>nd</sup> International Conferences on Supercomputing

1988 –, Editorial Board for *The International Journal of Supercomputer Applications and High Performance Computing*

1989 Planning Committee: 3<sup>rd</sup> International Conferences on Supercomputing

1989 review committees for the 5-year grant renewals of the Illinois, Pittsburgh and San Diego NSF Supercomputer Centers and chaired the San Diego panel

1990 Workshop team that helped design the Molecular Sciences Computing Facility at PNNL

1990 1988 Planning Committee: 4<sup>th</sup> International Conferences on Supercomputing

1990 Planning Committee for Supercomputer '90

1991-1995 Advisory Panel of the Molecular Science Computing Facility

1992 Symposium Organizer at the American Chemical Society National Spring meeting in San Francisco, "Applications of Numerical Simulations to Fluorine Chemistry."

1994-1995 Advisory Board of the Environmental Molecular Science Laboratory at the Pacific Northwest Laboratories

1993 Workshop to produce a white paper for DOE, NSF, and NIH on high performance computing needs in chemistry

1995 One of four non-Japanese participants in a MITI sponsored meeting on Japan on the design of new materials using supercomputers

1994-1997, Vice Chair for Programs, ACS Division of Fluorine Chemistry

1995-1997 Review Panel for the Chemistry Division of NIST

1998, Chair, ACS Division of Fluorine Chemistry

1997- 2002, Chair of Council of Chemical Research Subcommittee on Computational Chemistry for Vision 2020

1993- 1998, Editorial Advisory Board for *The Journal of Physical Chemistry*

1993-1995, Technical Advisory Board for Gaussian, Inc.

1990-1995, Technical Advisory Board for Biosym Technologies.

1996-1997, NRC Committee on Assessment of Fire Suppression Substitutes and Alternatives to Halon

1998 Co-organizer, BES workshop on “Research Frontiers in Molecular Simulation and Computational Chemistry: Extending the Accuracy and Scale of Molecular-Based Calculations,” Santa Fe, NM

1998 DOE Workshop on “Fundamental Challenges in Electron-Driven Chemistry”, Berkeley CA

2000-2002, DOE Chemical Sciences Council

2001 – 2011, DOE Geosciences Council member

2001 – 2003, Board of Fellows, PNNL/UW Joint Institutes

2002 – 2003, NIH Study Section on SBIR/STTR’s and instrumentation R01’s.

2003 DOE Office of Science workshop on the Science Case for Large-scale Simulation (ScaLes)

2003, U.S. Workshop on The Roadmap for the Revitalization of High-End Computing (HECRTF)

2005 Invited presentation and breakout session organizer, DOE Workshop “Advanced Fuel Cycle Initiative,” Gaithersburg, MD

2006 Invited participant, presentation, and writer at the DOE BES workshop: “Basic Research for Advanced Nuclear Energy Systems,” Bethesda, MD

2006 Invited participant, session organizer (Separations) and writer at the DOE OASCR workshop: “Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems,” Washington, DC

2007 Invited participant, session organizer (Research at Fundamental Scales) and writer at the DOE OASCR workshop: “Computational Subsurface Sciences,” Rockville MD

2007 Invited participant at the DOE BES workshop: Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems, Rockville MD

2007 Plenary lecturer and writer, DOE OASCR Workshop, “Computational Research Needs in Alternative and Renewable Energy,” Rockville MD

2007 Symposium Organizer at the American Chemical Society National Fall meeting in Boston, Division of Fuel Chemistry, “Hydrogen Storage and Fuel Cell Technology”.

2008 Symposium Organizer at the American Chemical Society National Spring meeting in New Orleans, Division of Fuel Chemistry, “Computational Methods and Modeling in Fuel Chemistry”.

2009 Co-organizer, Catalysis Science Program Meeting, Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic, Energy Sciences (OBES), U.S. Department of Energy, Annapolis, MD

2009 Co-lead writer for the 2010 EMSL MSCF Greenbook Section on Environmental Sciences, Workshop

2010 Co-organizer, DOE Basic Energy Sciences Geosciences Council Workshop “Computational Geochemistry: Predicting Properties of the Mineral-Water Interface” Annapolis, MD

2011 Organizer, 20<sup>th</sup> Winter Fluorine Conference, St. Petersburg Beach, FL

2011-2015, EMSL User Executive Committee, Pacific Northwest National Laboratory

2011-present, Editorial Advisory Board for *The Journal of Physical Chemistry*

2012-present, Editorial Board for *Journal of Fluorine Chemistry*

2013-present, Councilor, ACS Division of Fluorine Chemistry

2014-2015 ALCF (Argonne Leadership Computing Facility) User Advisory Council, Argonne National Laboratory

2014-present, OLCF (Oak Ridge Leadership Computing Facility) User Executive Board, Oak Ridge National Laboratory

2014-present, Editorial Board for *Computational and Theoretical Chemistry*

2015 Co-Organizer, 22<sup>nd</sup> Winter Fluorine Conference, St. Petersburg Beach, FL

2015, Organizer, ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur, Division of Fluorine Chemistry, 249<sup>th</sup> ACS National Meeting, Denver, March.

2015, Organizer, ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe, Division of Fluorine Chemistry, 249<sup>th</sup> ACS National Meeting, Denver, March.

2016-2018, ACS Joint Board-Council Committee on Publications (member), 2014-2015, Associate member)

#### **PhD Students (U. MN):**

Robert A. Eades (PhD, 1983), IBM Middle East and Africa

Mark Ellenberger (PhD, 1983) Independent Non-Profit Organization Management Professional, St. Paul, MN

Steven C. Richtsmeier (PhD, 1983) Principal Scientist, Spectral Sciences, Inc.

Robert Glinski (PhD, 1983), Prof., Chemistry, Tennessee Tech

David Weil (PhD, 1984) Applications Scientist at Agilent Technologies

#### **PhD students (UA):**

Keith Gutowski (PhD, 12/2006), Postdoc, Notre Dame, 2006-2008; BASF, 2008-

Raluca Craciun (PhD, 5/2010), Postdoc, St. Jude's Research hospital, 2010 – 2012; Assistant Professor, Department of Chemistry, Spring Hill College, 2012-2015; Visiting Assistant Professor of Chemistry, Division of Natural and Mathematical Sciences, LeMoyne-Owen College, 2015-

Daniel Grant (PhD, 8/2010), Postdoc, University of Minnesota, 2010-2012; Rustoleum, 2014-

Monica Vasiliu (PhD, 8/2010), Postdoc UA 2010-2016; Research Scientist, UA, 2016-

Tsang-Hsui Wang (PhD, 8/2010) R & D Chemist, Kimoto Tech Inc.

Jason Dyer (Masters, 2011) Associate Utility Engineer, Albany Water Dept., Georgia

Amanda Stott (PhD, 5/2012) CEO Tiki Bar Soap Co., MediaNet Software

Mingyang Chen (PhD, 8/2013) Postdoc, ORNL, 2013-2016; research assistant professor Beijing Computational Science Research Center (CSRC) 2016-

Virgil Jackson, (PhD, 12/2013) Postdoc UA, 2013-2015; Assistant Prof. Spring Hill College, 2015-

Zongtang Fang (PhD, 5/2014), Postdoc UA

Ted Garner (PhD, 8/2014), Samford Law School

Tanya Mikulas (PhD, 5/2015), Postdoc, University of Iowa

Michele Stover (PhD, 8/2015), Faculty, Louisiana School for Math, Science, and the Arts

Shengjie Zhang (4<sup>th</sup> year)

Luis Flores (4<sup>th</sup> year)

#### **Postdoctoral Fellows (PNNL):**

Giovanni Sandrone, 1998-1999, Italfarmaco Research Centre, Milan

Jorge Garza, 1998-2000, Profesor Titular C de Tiempo Completo, UAM-Iztapalapa

Rubicelia Vargas, 1998-2000, Profesor Titular C de Tiempo Completo, UAM-Iztapalapa

Chang-Guo Zhan, 2000-2003, Prof. Pharmaceutical Sciences, University of Kentucky

#### **Postdoctoral Fellows (UA):**

Shenggang Li, 2004-2011, Asst. Prof. Low-Carbon Conversion Center, Shanghai Advanced Research Institute, Chinese Academy of Sciences

Myrna Hernandez-Matus, 2005-2008, Profesor Titular C de Tiempo Completo, Universidad Veracruzana

Monica Vasiliu, 2010-present

Keijing Li, 2010, Lecturer, School of Chemical Engineering, East China University of Science and Technology, Shanghai

Kanchana (Sahan) Thanthiriwatt 2011-present

Mariano Mendez Chavez, 2013-present

Mingyang Chen, 2013 (see above)

Virgil Jackson, 2014-2015 (see above)

Zongtang Fang, 2014-present

### Visiting Faculty

Prof. M. T. Nguyen (K.U. Leuven), 9/2005-9/2009

Dr. Sadulla R. Allayarov, Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Chernogolovka, 8/2014-11/2014

### Undergraduate Research Students at UA (~50 total)

#### Current

*Shuwen Yue*, senior, CBHP, 3.5 year, Benchmarking catalytic reactions, Computational studies of models of the Schrock and Grubbs catalysts, 2014, 2015 Randall Research Award

*Sean Miller*, senior, Emerging Scholar, 3.0 year, Chemistry research, 1 year, Computational studies of phosphorylated amino acids, 2015 Randall Research Award

*Hayden Arnold*, junior, CBHP, 1.5 yr, computational studies of initial plutonium colloid formation

*Julia Murphy*, senior, 1.5 yr, Chemistry research, Carbonate formation from the reactions of CO<sub>2</sub> with transition metal oxides.

*Jonathan Belcher*, sophomore, 1.0 yr, Emerging Scholar, The Ethanol Condensation Reaction on M<sub>2</sub>O<sub>4</sub> (M=Ti, Zr, Hf ) Nanoclusters

*Will Jackson*, senior, 1.0 yr, Chemistry research, Gas-Phase Acidities of Acid-Substituted Dipeptides

*Michael Outlaw*, sophomore, CBHP, 0.5 yr, computational studies of catalysis

*Caroline Bloodworth*, sophomore, CBHP, 0.5 yr, computational studies of fluorocarbon thermochemistry

*William Layfield*, junior, CBHP, 0.5 yr, computational studies of actinides

*Emma Clements*, sophomore, CBHP, 0.5 yr, computational studies of actinides

*Laura Holland*, sophomore, 0.5 yr, computational studies of peptide chemistry

#### Former

*Blake Copeland*, 1.0 yr, junior, Chemistry research, Nitrate formation from the reactions of NO<sub>2</sub> with transition metal oxides

*Jacob Owen*, 0.5 yr, Chemistry research, Computational biochemistry, peptide acidities

*Sawyer Foyle*, junior, 1.0 year, Chemistry research, Ir carbonyl clusters with carbene ligands

*Cody Savage*, sophomore, 0.5 yr, Chemistry research, Gas-Phase Acidities of Phosphorylated Dipeptides

*Steven Spellmon*, Emerging Scholar, 1.5 year, Chemistry research, 1 year, Converting CO<sub>2</sub> to MeOH using Frustrated Lewis Pairs

*Patrick Zetterholm*, Emerging Scholar, 0.5 year, Computational Studies of Trimethylene Glycol Conversion on a (WO<sub>3</sub>)<sub>3</sub> Nanocluster

*Eric Terrell*, Emerging Scholar, 0.5 year, Role of Ligand Conformations in the Structure and Reactivity of Palladium-Phosphine Catalysts

*Maranda Burns*, CBHP, 0.5 year, Computational Studies of Gas-Phase Peptide Acidities and Decomposition Mechanisms

*Meredith Rickard*, 2.0 years, CBHP research, reduction of CO<sub>2</sub> using main-group catalysts, 2014, 2015 Randall Research Award

*Michael Raddatz*, 1 year, CBHP research, computational studies of gas-phase peptide acidities and decomposition mechanisms.

*Stephen Walker*, 3 years, CBHP + summer research, metal ion oxidation and reduction reactions in aqueous solution for carbon sequestration and nuclear fuel processing, Randall Research Award, Goldwater Scholar.

*Matt Outlaw*, 3 years, CBHP research + undergraduate research, photocatalytic reactions of transition metal oxide clusters for water splitting. 2 Randall Research Awards.

*Josh Moon*, 2 years, CBHP research, design of new synthons for inorganic materials - novel group IVB transition metal oxide clusters. Goldwater Scholar. Randall Award, Catherine J. Randall Award.

*Andrew Jones*, 2 years, CBHP research, prediction of the thermodynamics of key fuels and intermediates from biomass, Randall Award.

*J.T. Davis*, 2 years, CBHP research, acidities of peptides for negative ion proteomics, Randall Research Award

*Henk Both*, 1 year + 1 summer, CBHP research, benchmarking of the clustering energies and electron detachment energies of transition metal oxides, amino acid chemistry

*Ryan Flammerich*, 2 years, CBHP + summer research, actinide oxide cluster hydrolysis reactions, Randall Research Award, Truman Scholar

*Matthew Kelley*, 3 years, CBHP + summer research, oxidative dehydrogenation reactions of transition metal oxide clusters, Hollings Scholar, Goldwater Scholar, Randall Research Award (x3)

*Jessica Duke*, 3 years, CBHP + summer research, water reactions in carbon dioxide clusters for carbon sequestration, Hollings Scholar, Goldwater Scholar, Randall Research Award (x3), NSF Graduate Fellowship

*J. Pierce Robinson*, 3 years, CBHP research, hydrazine chemistry for regeneration of spent fuel for chemical hydrogen storage, Randall Research Award (x2)

*Kurt Guynn*, 2 years, CBHP research, thermochemistry of products derived from biomass, Randall Research Award

*Richard Cockrum*, 2+ years, thermochemistry of chemical weapons of mass destruction, Hollings Scholar, 2010 USA Today All-Academic 3<sup>rd</sup> Team, Randall Research Award

*Darryl (DJ) Outlaw*, 3 years, CBHP research, computational chemical hydrogen storage, Randall Research Award(x2), Catherine J. Randall Award

*Ashley McNeil* (Austin Peay State University), 3 months, summer REU, acidities of peptides for negative ion proteomics

*Kyle Smith* (Georgia Tech), 3 months, summer REU, reactions of transition metal oxide clusters

*Joni Corbin*, 6+ months, CBHP research, actinide hydrolysis

*Erica Schwalm*, 6+ months, CBHP research, single site transition metal catalyst

*Rebecca Long*, 3 yrs CBHP research, computational catalysis, transition metal bond energies, Randall Research Award(x2), Hollings Scholar, Goldwater Scholar, USA Today All Academic Honorable Mention 2010

*Nicollette Corbin* 5 months, CBHP research, actinide cluster thermochemistry

*Natalie Gist* 1.5 yr, CBHP research, catalysis with TiO<sub>2</sub> nanoparticles, Randall Research Award

*Jamie Hennigan*, 1.5+ yrs CBHP research, computational catalysis, transition metal thermochemistry, Randall Research Award, medical school, University of South Alabama



*Desiree Picone*, 2.0+ yrs CBHP research, computational catalysis, single metal sites in zeolites and transition metal electron affinities, Randall Research Award

*Michelle Stover (William Carey University)*, summer 2009, NSF REU student, amino acid acidities

*Courtney Guenther*, 1.0 yr, CBHP research, computational catalysis, Randall Research Award

*Jessica Kuperburg*, 1 semester, Spring 2009, Freshman research, amino acid acidities

*Mark Pinkerton*, 1 semester, Spring 2009, Freshman research, amino acid acidities

*Ashley Getwan*, 1 semester, Spring 2009, Freshman research, actinide chemistry

*Tyler Campbell*, 6 months, CBHP research, actinide hydrolysis reactions

*Emily Waymans*, 1.5 yr, CBHP research, TiO<sub>2</sub> chemistry and phosphine binding energies and cone angles for homogeneous catalysis, Hollings Scholar

*Maggie Adams*, 0.5 yr, CBHP research, amino acid acidities

*John Killian*, 1 + year, chemistry research, amino acid and peptide acidities

*Kevin Anderson*, 2 + years CBHP research, computational hydrogen storage, Randall Research Award

*Dan Marion* – 2.0+ yrs CBHP research, carbene chemistry – energetics and spectroscopy

*Jacob Batson*, 2.5 yrs CBHP research, computational hydrogen storage and computational biology (new project); 2<sup>nd</sup> place winner, College of Arts and Sciences undergraduate research presentations, April, 2005; Randall Research Award(x2)

*Ryan House*, CBHP, 2 yr + 2 summer semesters CBHP, computational catalysis; 3<sup>rd</sup> place winner, University of Alabama System Sciences undergraduate research presentations, April, 2006, Randall Research Award(x2)

*Glenn Kelly*, 3 yrs CBHP, computational catalysis; Randall Research Award(x3), Goldwater Scholar

*Jackson Switzer* 3 yr CBHP, computational hydrogen storage and computational work for Homeland Security Randall Research Award(x3), Hollings Scholar, Goldwater Scholar, USA Today All American Academic 2<sup>nd</sup> Team, 2008

*Andrew Vincent*, 3 yr CBHP, computational environmental geochemistry and catalysis, 2 years Randall Research Award, Goldwater Scholar

*Neil Shah*, 2.5 yrs CBHP research, computational environmental science and computational biology

*Patrick Keenum*, 2 yrs CBHP research + 1 summer (paid), computational environmental science and computational biology

*Will Schaffer*, 1 yr research, computational chemistry

*Amanda Holland*, 1.5 yrs CBHP, computational catalysis

*Hector Adam Velasquez*, REU, summer, 2005, University of South Alabama

*Ronita Foulkes*, MINT REU, summer, 2005, junior from Illinois State

*Claire Chisholm*, 1 semester CBHP, 2004

*Jason Spruell*, 1 yr CBHP, Senior thesis research, 2005, USA Today All American Academic 3<sup>rd</sup> Team, 2005, NSF Graduate Fellowship, Goldwater Scholar

*Charnita Peoples*, MINT REU, summer 2004, junior UA,

*Lesley Magee*, Chemistry REU, summer 2004, sophomore from Alcorn State  
*Lawrence Haselmaier, Jr.*, CBHP, Fall 2004

**Editor**

*Annual Reports in Computational Chemistry*, Vol. 11 (2015) and Vo. 12 (2016).

## Publications (Peer reviewed)

1. "Acidity, Basicity and Gas-Phase Ion Chemistry of Hydrogen Selenide by Cyclotron Resonance Spectroscopy," D. A. Dixon, D. Holtz, and J. L. Beauchamp, *Inorg. Chem.*, **1972**, *11*, 960-963. DOI: [10.1021/ic50111a008](https://doi.org/10.1021/ic50111a008)
2. "Localized Orbitals in Ethyl Ion and the Perturbation of Ethylene by a Proton. Reaction of Localized Orbitals," D. A. Dixon and W. N. Lipscomb, *J. Am. Chem. Soc.*, **1973**, *95*, 2853-2860. DOI: [10.1021/ja00790a019](https://doi.org/10.1021/ja00790a019)
3. "Computer Simulation of Kinetics by the Monte Carlo Technique," D. A. Dixon and R. H. Shafer, *J. Chem. Educ.* **1973**, *50*, 648-650. DOI: [10.1021/ed050p648](https://doi.org/10.1021/ed050p648)
4. "Search for the Br<sub>2</sub> + Cl<sub>2</sub> Exchange Reaction," D. A. Dixon, D. L. King, and D. R. Herschbach, *Faraday Discuss. Chem. Soc.*, **1973**, *55*, 375-376. DOI: [10.1039/DC9735500369](https://doi.org/10.1039/DC9735500369).
5. "Possibility of Singlet-Triplet Transitions in Oxygen Exchange Reactions," D. A. Dixon, D. D. Parrish, and D. R. Herschbach, *Faraday Discuss. Chem. Soc.* **1973**, *55*, 385-387. DOI: [10.1039/DC9735500369](https://doi.org/10.1039/DC9735500369)
6. "Localized Molecular Orbitals and Chemical Reactions. II. A Study of Three-Center Bond Formation in the Borane-Diborane Reaction," D. A. Dixon, I. P. Pepperberg, and W. N. Lipscomb, *J. Am. Chem. Soc.*, **1974**, *96*, 1325-1333. DOI: [10.1021/ja00812a011](https://doi.org/10.1021/ja00812a011)
7. "Localized Orbitals in Large Boron Hydrides. B<sub>16</sub>H<sub>20</sub> and Related Molecules," D. A. Dixon, D. A. Kleier, T. A. Halgren, and W. N. Lipscomb, *J. Am. Chem. Soc.*, **1974**, *96*, 2293-2295. DOI: [10.1021/ja00814a073](https://doi.org/10.1021/ja00814a073)
8. "Molecular Beam Chemistry. Facile Six-Center Reactions of Dimeric Chlorine with Bromine and with Hydrogen Iodide," D. L. King, D. A. Dixon, and D. R. Herschbach, *J. Am. Chem. Soc.*, **1974**, *96*, 3328-3330. DOI: [10.1021/ja00817a059](https://doi.org/10.1021/ja00817a059)
9. "Localized Molecular Orbitals for Polyatomic Molecules. II. Structural Relationships and Charge Distributions for Open Boron Hydrides and Carboranes," J. H. Hall, Jr., D. A. Dixon, D. A. Kleier, T. A. Halgren, L. D. Brown, and W. N. Lipscomb, *J. Am. Chem. Soc.*, **1975**, *97*, 4202-4213. DOI: [10.1021/ja00848a010](https://doi.org/10.1021/ja00848a010)
10. "Molecular Beam Chemistry. Reactions Exchanging van de Waals Bonds Among Three or More Halogen Molecules," D. A. Dixon and D. R. Herschbach, *J. Am. Chem. Soc.*, **1975**, *97*, 6268-6270. DOI: [10.1021/ja00854a067](https://doi.org/10.1021/ja00854a067)
11. "Localized Molecular Orbitals for Polyatomic Molecules. III. Monocyclic Aromatic Rings," D. A. Kleier, D. A. Dixon, and W. N. Lipscomb, *Theoret. Chim. Acta*, **1975**, *40*, 33-45. DOI: [10.1007/BF00547911](https://doi.org/10.1007/BF00547911)
12. "Localized Molecular Orbitals for Polyatomic Molecules. IV. Large Boron Hydrides," D. A. Dixon, D. A. Kleier, T. A. Halgren, and W. N. Lipscomb, *J. Am. Chem. Soc.*, **1976**, *98*, 2086-2096. DOI: [10.1021/ja00424a012](https://doi.org/10.1021/ja00424a012)
13. "Electronic Structure and Bonding of the Amino Acids Containing First Row Atoms," D. A. Dixon and W. N. Lipscomb, *J. Biol. Chem.* **1976**, *251*, 5992-6000.

<http://www.jbc.org/content/251/19/5992.abstract?sid=c47eb8c5-5591-45b4-88f7-42e0fda384df>

14. "Potential Energy Surface for Bond Exchange Among Three Hydrogen Molecules," D. A. Dixon, R. M. Stevens, and D. R. Herschbach, *Faraday Discuss. Chem. Soc.*, **1977**, 62, 110-126. DOI: [10.1039/DC9776200110](https://doi.org/10.1039/DC9776200110)
15. "Ab Initio Study of the Electronic Structure of  $\text{Li}_2^-$ ," D. A. Dixon, J. L. Gole, and K. D. Jordan, *J. Chem. Phys.*, **1977**, 66, 567-572. DOI: [10.1063/1.433978](https://doi.org/10.1063/1.433978)
16. "Theoretical Studies of Inversion Barriers in Pyramidal Molecules," D. S. Marynick and D. A. Dixon, *Faraday Discuss. Chem. Soc.*, **1977**, 62, 47. DOI: [10.1039/DC9776200047](https://doi.org/10.1039/DC9776200047)
17. "Energy Transfer Processes Involving van der Waals Bonds," D. A. Dixon and D. R. Herschbach, *Ber. Bunsenges. Phys. Chem.*, **1977**, 81, 145-150. DOI: [10.1002/bbpc.19770810211](https://doi.org/10.1002/bbpc.19770810211)
18. "Inelastic Energy Transfer in Chlorine Dimers," D. A. Dixon and D. R. Herschbach, *Faraday Discuss. Chem. Soc.*, **1977**, 62, 309. DOI: [10.1039/DC9776200300](https://doi.org/10.1039/DC9776200300)
19. "Lifetime for Predissociation of Vibrationally Excited van der Waals Molecules," D. A. Dixon, D. R. Herschbach, and W. Klemperer, *Faraday Discuss. Chem. Soc.*, **1977**, 62, 341-343. DOI: [10.1039/DC9776200300](https://doi.org/10.1039/DC9776200300)
20. "Six-Center Reaction Systems:  $\text{H}_6$ ,  $\text{H}_2\text{Li}_4$ , and  $\text{Cl}_6$ ," D. A. Dixon and D. R. Herschbach, *Faraday Discuss. Chem. Soc.*, **1977**, 62, 162-166. DOI: [10.1039/DC9776200138](https://doi.org/10.1039/DC9776200138)
21. "The Bond Energy-Bond Order Method," D. A. Dixon and D. R. Herschbach, *Faraday Discuss. Chem. Soc.*, **1977**, 62, 166-168. DOI: [10.1039/DC9776200138](https://doi.org/10.1039/DC9776200138)
22. "Limitations of Molecular Orbital Correlations for Reactions," D. A. Dixon and D. R. Herschbach, *Faraday Discuss. Chem. Soc.*, **1977**, 62, 343-345. DOI: [10.1039/DC9776200300](https://doi.org/10.1039/DC9776200300)
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677. “A Practical Guide to Reliable First Principles Computational Thermochemistry Predictions Across the Periodic Table,” D. A. Dixon, D. Feller, and K. A. Peterson, in

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681. "The Impact of Larger Basis Sets and Explicitly Correlated Coupled Cluster Theory on the Feller-Peterson-Dixon Composite Method," D. Feller, K. A. Peterson, and D. A. Dixon in *Annual Reports in Computational Chemistry*, Vol. 12, ed. D. A. Dixon, Elsevier, Amsterdam, 2016, accepted, in press.
682. "Ab initio calculations," D. A. Dixon, in *Earth Sciences Series. Encyclopedia of Geochemistry*, Ed. W. W. White, Section Ed. W. H. Casey, Springer, in press, 2016.
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### **Books Edited**

686. *Annual Reports in Computational Chemistry, Vol. 11*, D. A. Dixon, Ed. Elsevier, Amsterdam, 2015. 6 chapters. ISBN: 978-0-444-63710-9
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### **Proceedings Contributions and extended preprints**

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691. "Numerical Simulation of Molecular Properties in the Chemistry Industry," D. A. Dixon in *Science and Engineering on Cray Supercomputers, Proceedings of the Third International Symposium*, Cray Research, Inc. Minneapolis, MN 1987, p. 169-193.
692. "Supercomputer Applications in the Chemical Industry," D. A. Dixon in *Proceedings of the Second International Conference on Supercomputing*, ed. L. P. and S. I. Kartashev, International Supercomputing Institute, St. Petersburg, FL (1987) Vol. II, p. 329-334.
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696. "Visualization and Quantum Chemistry" D. A. Dixon, P. J. Capobianco, J. E. Mertz, and E. Wimmer, in *Science and Engineering on Cray Supercomputers. Proceedings of the Fourth International Symposium*, Cray Research, Minneapolis, MN 1988, 189-208.
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704. "The Prediction of Molecular Properties for Product Life Cycles," D.A. Dixon, K.D. Dobbs, M. Neurock, J. Lerou, and T. Nakao *Proceedings of the 9th International Symposium on Large Chemical Plants*, Antwerp, Belgium **1995**, pp.101-138
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706. "The 21<sup>st</sup> Century: How Far Can COMP Go with the Hardest Problems?" D.A. Dixon, Book of Abstracts, Division of Computers in Chemistry, ACS National Meeting, San Francisco, CA, March 26-30, 2000, American Chemical Society, Washington DC, **2000**, pp. 12-15
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712. "High Accuracy Computational Studies of Boron-Nitrogen Compounds for Chemical Hydrogen Storage," M. H. Matus, D J. Grant, S. V Nguyen, K. D. Anderson, M. T. Nguyen,

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717. "Active Nanostructures at Interfaces for Photocatalytic Reactors and Low-power Consumption Sensors," J. L. Gole, S. Ozdemir, S.M. Prokes, and Dixon, D.A., *MRS Proceedings*, **2010**, 1257-009-04 (6 pages)
718. "Computational Studies of the NiTi Alloy System: Bulk, Supercell, and Surface Calculations," A. C. Stott, P. B. Abel, C. DellaCorte, S. V. Pepper, and D. A. Dixon, *MRS Proceedings*, **2011**, 1295, 15-20

### Book reviews

719. Review of "Current Methods on Inorganic Chemistry. Volume 1. Theoretical Methods of Molecular Magnetism," D.A. Dixon, *J. Am. Chem. Soc.*, **2000**, 122, 8806. DOI: 10.1021/ja995800s
720. Review of *Advances in Chemical Physics*. Vol. 126, Ed. I. Prigogine (The University of Texas-Austin and Université Libre de Bruxelles) and Stuart A. Rice (The University of Chicago). John Wiley & Sons, Inc.: Hoboken, NJ. 2003. x + 306 pp. ISBN 0-471-23582-2. Dixon, D. A. *J. Am. Chem. Soc.* **2003**, 125, 14952. DOI: 10.1021/ja033544k
721. Review of *Computational Mechanisms of Au and Pt Catalyzed Reactions*. Edited by Elena Soriano and José Marco-Contelles (Instituto de Química Orgánica General, Madrid, Spain). From the series, Topics in Current Chemistry, 302. Springer: Heidelberg, Dordrecht, London, New York. 2011. xiv + 252 pp. \$309. ISBN: 978-3-642-21082-2. *J. Am. Chem. Soc.*, **2011**, 133, 19257. DOI: 10.1021/ja2099694

### Corporate journals

722. "Molecular Modeling of Polymeric Materials Using Ab Initio Molecular Orbital Theory," D. A. Dixon in *Chemical Automation News*, Polygen, Waltham, MA (May, **1987**) Vol. 2, No. 5, p. 1.
723. "Economic Benefits of Large Scale Numerical Simulation", D. A. Dixon in *Chemical Automation News*, Polygen, Waltham, MA (Sept. **1988**) Vol. 3, No. 9, p. 1.

724. "Computational Chemical Design of CFC Alternatives at DuPont", D. A. Dixon, K. D. Dobbs, and S. C. Walker, *Cray Channels*, **1994**, *16*, No. 1, 7-11.

### **Patents**

"Spherical carbonaceous material, device using it, and its manufacture," Inventor (Author): Matsuzawa, Nobuyuki; Dixon, David A.; Masafumi, Ata; Nobutoshi, Asai, Assignee: E. I. Du Pont de Nemours and Co.; SONY Corp. Patent: Japan Kokai Tokkyo Koho; JP 96337409 A2; JP 08337409; Date: 1996.12.24; Application: JP 95167992 (19950609)

"Metallocene nonlinear optical material and device using it," Inventor (Author): Matsuzawa, Nobuyuki; Dixon, David A.; Nobutoshi, Asai, Assignee: E. I. Du Pont de Nemours and Co.; SONY Corp., Patent: Japan Kokai Tokkyo Koho; JP 96338999 A2; JP 08338999, Date: 1996.12.24, Application: JP 95167993 (19950609)

"Metal phthalocyanine or porphyrin nonlinear optical material and device using it," Inventor (Author): Matsuzawa, Nobuyuki; Dixon, David A.; Kishii, Noriyuki, Assignee: E. I. Du Pont de Nemours and Co.; SONY Corp., Patent: Japan Kokai Tokkyo Koho; JP 96339000 A2; JP 08339000, Date: 1996.12.24, Application: JP 95167994 (19950609)

## Invited Lectures

1. University of California, Berkeley, Physical Chemistry Seminar, Feb. 1975.
2. Harvard University, Organic Chemistry Seminar, Oct. 1975.
3. Battelle Memorial Institute, Columbus, Ohio, Seminar, Nov. 1975.
4. Harvard University, Physical Chemistry Seminar, May 1976.
5. California Institute of Technology, Physical Chemistry Seminar, May 1977.
6. California State University at Los Angeles, Chemistry Seminar, May 1977.
7. Los Alamos Scientific Laboratory, two seminars, May 1977.
8. Georgia Institute of Technology, Physical Chemistry Seminar, Oct. 1978.
9. Drake University, Chemistry Seminar, Jan. 1979.
10. University of Wisconsin, Milwaukee, Physical Chemistry Seminar, Nov. 1979.
11. Argonne National Laboratory, Chemistry Division, Seminar, Mar. 1980.
12. ACS Meeting, Atlanta, Invited Lecture: High Temperature Chemistry Symposium, Apr. 1981.
13. Harvard University, Physical Chemistry Seminar, Apr. 1981.
14. Brandeis University, Physical Chemistry Seminar, Apr. 1981.
15. Gordon Conference on Infra-red Intensities, Invited Lecture, Portsmouth, NH, June 1981.
16. Georgia Institute of Technology, Physical Chemistry Seminar, Sept. 1981.
17. Drake University, Chemistry Seminar, Jan. 1982.
18. Stanford University, Physical Chemistry Seminar, Mar. 1982.
19. Polyatomics Research/NASA-Ames, Seminar, Aug. 1982
20. University of Pittsburgh, Physical Chemistry Seminar, Sept. 1982.
21. 41st International Pittsburgh Diffraction Conference and 3rd Canadian Crystallography Conference, Invited Lecture, Pittsburgh, PA, Oct. 1983.
22. University of British Columbia, Chemistry Department Seminar, Nov. 1983.
23. Lehigh University, Chemistry Department Seminar, Nov. 1983.

24. Harvard University, Organic Chemistry Seminar, Mar. 1984.
25. Brandeis University, Physical/Organic Chemistry Seminar, Mar. 1984
26. University of Delaware, Physical Chemistry Seminar, Apr. 1984,
27. Invited Speaker, 1984, International Chemical Congress of Pacific Basic Societies (Pacifichem), Nobel Laureate Symposium on Applied Quantum Chemistry, Honolulu, Hawaii, Dec. 1984.
28. Invited Speaker, 7th Winter Fluorine Conference, Orlando, Florida, Feb. 1985.
29. University of Virginia, Charlottesville, Physical Chemistry Seminar, Feb. 1985
30. Invited Lecturer, CRAY Research Science and Engineering Symposium, Minneapolis, Apr. 1985.
31. Invited Lecturer, Gordon Conference on "Physical Organic Chemistry," June 1985.
32. Southern Illinois University, Physical Chemistry Seminar, Nov. 1985.
33. Invited Lecture, MEDCOMP Southeast, University of Georgia, Dec. 1985.
34. University of Georgia, Chemistry Department Seminar, Feb. 1986.
35. Georgia Institute of Technology, Chemistry Department Seminar, Feb, 1986.
36. Invited Lecture, Fluorine Division, ACS National Meeting, Apr. 1986.
37. Invited Lecture, CRAY Symposium on Supercomputers in Chemistry, Minneapolis, June 1986 and Lausanne, Sept. 1986.
38. NASA/Ames Moffet Field Seminar, July 1986.
39. University of California, Berkeley, Physical Chemistry Seminar, July 1986.
40. Max Planck Institute fur Astrophysics, Munich, Seminar, Sept. 1986.
41. North Texas State, Denton, Chemistry Seminar, Jan. 1987.
42. University of Texas, Arlington, Chemistry Seminar, Jan. 1987.
43. Invited Lecture, 8th Winter Fluorine Conference, St. Petersburg, Florida, Jan. 1987.
44. Vanderbilt University, Chemistry Department, seminar, Feb. 1987.
45. Invited lecture, FCCSET Workshop on Research in Large-Scale Computational Science and Engineering, Feb. 1987



46. Invited Lecture, ACS National meeting, James Flack Norris Award Symposium for Paul v. R. Schleyer, Organic Division, Denver, Apr. 1987.
47. Invited Lecture, ACS National meeting, "Symposium on Supercomputer Applications in Chemistry," Physical Division, Denver, Apr. 1987.
48. Invited Lecture, ACS National meeting, "Metals in Organic Synthesis," Inorganic Division, Denver, Apr. 1987.
49. Georgia Institute of Technology, Chemistry Department, seminar, Apr. 1987
50. Symposium Organizer/Lecturer, 2nd International Conference on Supercomputing, "Computational Chemistry on Supercomputers" Santa Clara, May 1987.
51. EMRC Invitational Lecture Series, Allied-Signal, Chicago, June 1987,
52. Invited Lecture, National Computer Conference, "Minisymposium on Supercomputer Applications" Chicago, June 1987.
53. Invited Lecture, Third International Science and Engineering Symposium on CRAY Supercomputers, Minneapolis, MN, Sept. 1987.
54. Invited Lecture, 40th Gaseous Electronics Conference, Georgia Tech, Oct. 1987.
55. University of Georgia, Chemistry Department Seminar, Oct. 1987.
56. Invited Lecture, 28th Sanibel Symposium, Marineland, FL, March 1988.
57. Lecture, Organizer/Chair, Computational Chemistry Symposium, Third International Conference on Supercomputing, Boston, MA, May 1988.
58. Invited Lecture, ACS National Meeting, Division of Fluorine Chemistry, "Fluoropolymer Symposium Honoring 50th Anniversary of the Discovery of Teflon" Toronto, June 1988.
59. Invited Lecture, ACS National Meeting, Division of Polymeric Materials, Science and Engineering "Symposium on Computer Applications in Applied Polymer Science" Toronto, June 1988.
60. Invited Lecture, Symposium on Computational Chemistry on CRAY Supercomputers, Tokyo, Japan, July 1988.
61. Invited Lecture, International Fluorine Conference, University of Santa Cruz, August 1988.
62. Invited Lecture, First Ohio Supercomputer Symposium, Ohio State University, Sept. 1988.
63. Invited Lecture, 2nd Symposium on Computational Chemistry on CRAY Supercomputers, Chicago, IL, Sept. 1988

64. Invited Lecture, Fourth International Symposium on Science and Engineering on CRAY Supercomputers, Minneapolis, MN, Oct. 1988.
65. Invited Lecture, Grand Challenges in Computational Science, Molokai, HI, Jan. 1989.
66. Invited Lecture, 9th Winter Fluorine Conference, St. Petersburg, FL, Jan. 1989.
67. Invited Lecture, ACS National Meeting, Dallas, TX, Apr. 1989.
68. Invited Lecture, Fourth International Symposium on Supercomputing, Santa Clara, CA, May, 1989
69. Invited Lecture, CRAY Symposium on Supercomputing, Washington, D.C. May, 1989.
70. IBM Research-Almaden, Seminar, San Jose, CA, July, 1989
71. Invited Lecture, AIChE National Meeting, Philadelphia, PA, August, 1989
72. Invited Lecture, Ohio State Industrial Affiliates Symposium, Columbus, OH., September, 1989
73. Wright-Patterson AFB, Seminar, Dayton, OH, Sept. 1989
74. Baekeland Award Symposium, Lecture and Award Address, Hoffman-LaRoche, Nutley, NJ, October 1989
75. Invited Lecture, Supercomputing '89, Reno, NV, November 1989
76. Invited Lecture, Du Pont/University of Delaware Symposium on Numerical Simulation, Newark, DE, Dec. 1989
77. Invited lecture and Co-organizer of symposium, Pacificchem Honolulu HI, Dec. 1989
78. Invited lecture, Pacificchem Honolulu HI, Dec. 1989
79. University of Montreal, Chemistry Department, seminar, Jan. 1990.
80. Invited Lecture, ACS National Meeting, Fluorine Symposium, Boston, MA, Apr. 1990.
81. Invited Lecture, "Chemical Applications of Local Density Functional Theory", Ohio Supercomputer Center, May 1990.
82. Invited Lecture, Sandia Livermore National Laboratory, Albuquerque, NM, May 1990.
83. Invited Lecture, Symposium on Semi-Empirical Methods, World Association of Theoretical Organic Chemists, Toronto, July 1990.
84. Invited Panelist at SIGGRAPH '90, Dallas, Aug., 1990.

85. Invited Lecture, North Carolina ACS Symposium on Computational Chemistry, North Carolina State University, Sept. 1990.
86. Invited Lecture, INEL Symposium on Computing, Idaho Falls, ID, Sept. 1990.
87. Invited Lecture, Fifth Cray Science and Engineering Symposium, London, England, Oct. 1990
88. Invited Lecture, NATO ASI on Molecular Magnetism, Il Ciocco, Italy, Oct. 1990.
89. Chemistry Department SUNY Albany, Seminar, Nov. 1990.
90. Invited Lecture, Cray Chemistry Symposium, Tokyo, Japan, Dec. 1990.
91. Invited Lecture, Cray Chemistry Symposium, Kobe, Japan, Dec. 1990
92. Invited Lecture, Tenth Winter Fluorine Conference, St. Petersburg, FL, Jan. 1991.
93. Invited Lecture, Sanibel Conference on Quantum Chemistry, St. Augustine, FL, Mar. 1991.
94. Invited Lecture, Computational Aspects of Materials Research, Queens University, Canada, May 1991.
95. Invited Lecture, Cray Chemistry Symposium, Minneapolis, MN, June 1991.
96. Invited Lecture, IBM European Summer School in Computational Chemistry, Oberlech, Austria, July 1991.
97. Invited Lecture, National AICHE Meeting, Pittsburgh, PA, Aug. 1991.
98. Invited Lecture, W.R. Grace Research Center, Washington, D.C. Aug. 1991.
99. Keynote speaker, Biosym Technologies Chemistry Symposia, Tokyo, Nov. 1991.
100. Keynote speaker, Biosym Technologies Chemistry Symposia, Osaka, Nov. 1991
101. Invited Lecture, EPA Laboratories, Duluth, MN, Feb. 1992
102. Organizer and Lecture, ACS National Meeting, Symposium on Computational Methods in Fluorine Chemistry, San Francisco, CA, Apr. 1992
103. Invited Lecture, Supercomputer Japan 1992, Yokohama, Apr. 1992
104. Invited Lecture, IBM Technical Executive Forum, Palm Springs, Apr. 1992.
105. University of Delaware, Chemistry Department, seminar, May 1992.

106. Invited Lecture, IBM European Summer School on Computer-Aided Chemistry for Molecular Properties and Molecular Design, Oberlech, Austria, July 1992
107. North Carolina State, Chemistry Department, seminar, Raleigh, NC Aug. 1992.
108. Invited Computational Chemistry Seminar, Ohio Supercomputer Center, Columbus, Sept. 1992
109. Invited seminar, Akzo (Arnhem), Netherlands, Oct. 1992
110. Invited seminar, KSLA (Shell Labs, Amsterdam), Netherlands Oct. 1992.
111. Invited seminar, Bayer (Leverkusen), Germany, Oct. 1992.
112. Invited Lecture, Cray European Chemical Executive Seminar, London, Dec. 1992
113. Invited seminar, Hoechst (Frankfurt), Germany, Dec. 1992
114. Invited seminar, BASF (Ludwigshafen), Germany, Dec. 1992
115. Invited Lecture, ACS Winter Fluorine Conference, St. Petersburg, FL, Jan. 1993.
116. Invited Lecture, U.S. Government Workshop on Computational Chemistry, NIH, Bethesda, MD, Mar. 1993
117. Invited Lecture, AIChE Spring National Meeting, Houston March, 1993.
118. Invited Panelist, U.S. Government, HPCI Grand Challenge Workshop, Industrial Panel, Pittsburgh, May 1993.
119. Invited Lecture, NIST Industrial Computational Chemistry Workshop, Gaithersburg, MD, May 1993
120. Invited Lecture, ASPRONC 17th Seminar on Frontier Technology, Tokyo and Oiso, Japan, May 1993.
121. Invited Lecture, ASPRONC 17th Seminar on Frontier Technology, Tokyo, Japan, May 1993
122. Invited Lecture, ASPRONC 17th Seminar on Frontier Technology, Oiso, Japan, May 1993
123. Invited Lecture, Asahi Glass, Japan, May/June, 1993.
124. Invited Lecture, Sumitomo Chemicals, Japan, May/June, 1993.
125. Invited Lecture, Nissan, Japan, May/June, 1993
126. Invited Lecture, Sony, Yokohama, Japan, May/June, 1993

127. Invited lecture at ARCO Research Center, Newtown Square, PA, July 1993.
128. Invited Lecture, National ACS Meeting, Chicago, Aug. 1993.
129. Invited Lecture, National ACS Meeting, Chicago, Aug. 1993
130. Invited Lecture, Ecochem Section, IUMRS, Tokyo, Japan, Sept, 1993
131. Invited Lecture, Sony, Japan, Sept. 1993.
132. Invited Lecture, Toshiba, Japan, Sept. 1993
133. Invited Lecture, Matsushita, Japan, Sept. 1993
134. Invited Lecture, Hitachi, Japan, Sept. 1993
135. Invited Lecture, Kao, Japan, Sept. 1993.
136. Invited Lecture, Kaneka, Japan, Sept. 1993
137. Invited Lecture, Sumitomo Electric, Japan, Sept. 1993.
138. Invited Lecture, Mitsui-DuPont Fluorochemicals, Japan, Sept. 1993
139. Invited Lecture, INEL Computing Symposium, Idaho Falls, ID, Oct. 1993.
140. Invited Lecture, Jackson State/U.S. Army Recent Advances in Computational Chemistry Symposium, Vicksburg, MI, Nov. 1993.
141. University of Pennsylvania, Physical Chemistry Seminar, Philadelphia, PA, Nov. 1993.
142. Invited Lecture, Supercomputing '93, Portland, OR, Nov. 1993.
143. Invited Lecture, National ACS Meeting, Michael J. Dewar Symposium, San Diego, CA, March 1994.
144. Plenary Lecture, DOE Catalyst by Design Meeting, Washington, D.C., April 1994.
145. Invited Lecture, 2nd Canadian Computational Chemistry Conference, Kingston, Canada, May 1994.
146. Invited lecture, DOE Catalyst and Surface Science Meeting, Oconowonomoc, WI, May 1994.
147. Invited Lecture, 30 Years of Density Functional Theory, Cracow, Poland, June 1994.
148. Invited Seminar, University of Singapore, Singapore, July 1994.

149. Invited Lecture, International Conference on Fluorine Chemistry, Kyoto, Japan, July 1994.
150. Invited Seminar, Chemistry Department, Iowa State University, Ames, IA, Sept. 1994.
151. Invited Seminar, Chemistry Department, University of Iowa, Iowa City, IA, Sept 1994.
152. Invited Lecture, Symposium on Computations on Supercomputers in the Chemical Industry, Bayer, Leverkusen, Germany, Oct. 1994.
153. Invited Lecture, American Institute of Chemical Engineers National Meeting, Symposium on Computational Chemistry in Industry, Nov. 1994.
154. Invited Seminar, Pacific Northwest Laboratory, Richland, WA, Jan. 1995.
155. Invited Lecture, 12th Winter Fluorine Conference, Jan. 1995.
156. Invited Lecture, MIT/Biosym Workshop on "The Impact of Molecular Modeling on Industrial Research," MIT, Cambridge, MA, April 1995.
157. Invited Lecture, 27th Central Regional Meeting of the ACS, May 1995.
158. Invited Lecture and co-organizer, CECAM Workshop, "Density Functional Methods in Chemistry--Assessment and Opportunities," Lyon, France, June 1995.
159. 2 Invited Lectures, NATO ASI on Ion-Molecule Chemistry, Garmisch-Partenkirchen, Germany, Aug. 1995.
160. Invited Lecture, Physical Chemistry Division, National ACS Meeting, Chicago, IL, Aug. 1995.
161. Plenary Lecture, Europort Meeting, "New Frontiers in Computational Chemistry: Impact of Parallel Computing on the Chemical and Pharmaceutical Industry," Strasbourg, France, Nov. 1995.
162. Invited Lecture, Pacifichem Meeting, Honolulu, HI, Dec. 1995.
163. Invited Lecture, Pacifichem Meeting, Honolulu, HI, Dec. 1995
164. Invited Lecture, Chemistry Department Texas A&M University, College Station, TX, Feb. 1996.
165. Invited Lecture, ACS National Meeting, Inorganic Fluorine Konrad Seppelt Award Symposium, New Orleans, Mar. 1996.
166. University of Washington, Physical Chemistry Seminar, Seattle, WA, May 1996.
167. Invited Lecture, ACS National Meeting, Computational Thermochemistry Symposium, Orlando, FL, Aug. 1996.

168. Invited Lecture, IBM Environmental Conference, Almaden, CA, Oct 1996.
169. Invited Lecture, 13th Winter Fluorine Conference in St. Petersburg, FL, Jan. 1997.
170. Invited Lecture, University of Utah Chemistry Department, SLC , UT, Mar. 1997.
171. Invited Lecture, Spring ACS Meeting in San Francisco, CA, Apr. 1997.
172. Invited presentation “Aspects of Electronic Structure Theory for Materials Design,” at the DOE/BES From Materials to Molecules Workshop in Austin, TX, Apr. 1997.
173. Invited presentation, AFEAS Meeting on HFC-134a Decomposition in Washington DC , May, 1997.
174. Invited presentation, Clean Products and Processes Conference, San Diego, CA, June 1997.
175. Invited Lecture, 9th International Congress of Quantum Chemistry Conference in Atlanta, GA, June 1997.
176. Invited Lecture, 15<sup>th</sup> International Symposium on Fluorine Chemistry in Vancouver, BC, Aug. 1997.
177. Invited Lecture, 5<sup>th</sup> Chemical Congress of North America Conference in Cancun, Mexico, Nov. 1997.
178. Invited Lecturer, 20th Anniversary Celebration, Chemistry Department, Autonomous Metropolitan University (UAM), Mexico City, Nov. 1997.
179. Invited Lecture, Stevens Institute of Technology, Hoboken, NJ, Dec. 1997.
180. Invited lecture, HPCI Conference 98, University of Manchester, Manchester, England, January, 1998.
181. Co-organizer and presenter, Computational Chemistry Technology Roadmap Workshop, DOE/OIT, University of Maryland, March 1998.
182. Invited presentation, IMP Symposium on Computational Science and Engineering, Mexico City, April 1998.
183. Invited Presentation, Photochemical Reactivity Workshop, EPA, Durham, NC, May, 1998
184. Invited presentation, 6<sup>th</sup> Boron USA Workshop, Athens, GA, May, 1998.
185. Invited presentation, Photochemical Reactivity Workshop, EPA, Durham, NC, May, 1998
186. Invited presentation, West Coast Theory Conference, Richland WA, June 1998.

187. Invited Lecture, 13<sup>th</sup> Canadian Symposium on Theoretical Chemistry, Vancouver, BC, Aug. 1998.
188. Invited Lecture, ACS National meeting, Schrobilgen Fluorine Award Symposium Aug. 1998.
189. Invited lecture, 15<sup>th</sup> International Symposium on Chemical Reaction Engineering, Newport Beach, CA, Sept. 1998.
190. Invited presentation, National Research Council's Chemical Sciences Roundtable workshop on "The Impact of Advances in Computing and Communications Technologies on Chemical Sciences and Technology," Washington, DC, Nov., 1998.
191. Invited presentation, Applied Mathematics Center, UNAM, Mexico City, Nov. 1998.
192. Invited seminar, Catalyst Center, Northwestern University, Nov. 1998.
193. Invited seminar, Elf-Atochem, King of Prussia, PA, Dec. 1998.
194. Invited lecture, 14th Winter Fluorine Conference in St. Petersburg, FL, Jan. 1999.
195. Invited Presentation, NSF Workshop, "Vision for Nanotech R&D in the Next Decade", Arlington, VA, Jan, 1999.
196. Invited lecture, U.S./Latin American/Canadian/Caribbean Workshop, "Molecular and Materials Sciences: Theoretical and Computational Aspects," Cuernavaca, Mexico, Feb. 1999.
197. Invited lecture, ACS National Meeting, Anaheim, CA, Mar. 1999
198. Invited lecture, ACS National Meeting, Anaheim, CA, Mar. 1999
199. ACS Chemistry and Chemical Engineering Lecturer, University of Wisconsin-Madison, Madison WI, Apr. 1999
200. Invited Lecture, BIO 99, Seattle, WA, May, 1999.
201. Invited presentation, DOE Workshop on Carbon Management, Santa Fe, NM, May, 1999.
202. Invited Presentation, III Congress of the International Society of Chemical Physics, Mexico City, Nov., 1999
203. Invited Lecture, Dow Chemical Company, Midland, MI, Nov. 1999.
204. Invited Lecture, Hilton Head Workshop on Computational Biology, Feb. 2000.
205. Invited Lecture, ACS National Meeting San Francisco, March 2000.



206. Invited Lecture, ACS National Meeting San Francisco, March 2000
207. Co-organizer and lecture, Sun Symposium on Computational Biology, May, 2000.
208. Invited Lecture, 2000 Northwest & Rocky Mountain ACS Joint Regional Meeting in Idaho Falls ID, June 2000
209. Invited Lecture and co-organizer, CCR NICHE Conference - Computational Chemistry & Fluid Dynamics in Marco Island FL, June 2000
210. Invited Lecture, 220th ACS National Meeting in Washington DC, US, August, 2000.
211. Invited Lecture, 220th ACS National Meeting in Washington DC, US, August, 2000
212. Invited Lecture, Computational Chemistry Gordon Conference, Oxford, ENGLAND, July, 2000.
213. Invited lecture, NETL, Pittsburgh, July, 2000.
214. Invited Lecture, PacifiChem 2000, Symposium on Inorganic Fluorine Chemistry, Honolulu, HI, Dec. 2000
215. Invited Lecture, PacifiChem 2000, Symposium on Applied Quantum Chemistry, Honolulu, HI, Dec. 2000
216. Invited lecture, 14th Winter Fluorine Conference in St. Petersburg, FL, Jan. 2001.
217. Invited Lecture, Symposium on Modeling, Society of Toxicology, Annual Meeting, San Francisco, March, 2001.
218. Invited Lecture, 2<sup>nd</sup> International Symposium on 157 nm Lithography, Dana Point CA, May, 2001.
219. Invited Lecture, "Gordon Conference on Biomolecules in the Gas Phase," New London, CT, June, 2001.
220. Invited Lectures, Autonomous University of Morelia, Cuernavaca, Mexico, August, 2001.
221. Invited presentation, DOE workshop on GTL Computational Research Priorities and Infrastructure Needs, Germantown, August, 2001.
222. Invited Talk, Sematech Photoresist Advisory Group meeting, Dallas, TX, January 2002
223. Invited talk, DOE Workshop on Mathematical Needs for Genomes to Life, Washington, DC, March, 2002
224. Invited lecture, Saxon Professorship Investiture of Anthony Arduengo, University of Alabama, May, 2002.

225. Invited lecture, Cambridge Healthtech Institute on Biological Systems Modeling, San Diego, CA June, 2002.
226. Invited presentation, DOE High Performance Network Planning Workshop, Washington, DC, Aug. 2002
227. Invited lecture, National ACS meeting, Boston MA, August, 2002.
228. Invited lecture, National ACS meeting, Boston MA, August, 2002
229. Invited Lecture, DOE Contractors meeting and workshop, Homogeneous Catalysis, Chicago, IL, Sept. 2002
230. Invited Lecture, NRC Workshop on the Environment, "Challenges for the Chemical Sciences in the 21<sup>st</sup> Century, Irvine, CA, Nov. 2002.
231. Invited Panelist, Supercomputing 2002, SC2002 Panel on Desktop Grids, Baltimore, MD, Nov. 2002.
232. Invited Lecture, Winter Fluorine Conference, St. Petersburg Beach FL, Jan. 2003
233. Award Address for the 2003 American Chemical Society Award for Creative Work in Fluorine Chemistry, 15<sup>th</sup> Winter Fluorine Conference, St. Petersburg Beach FL, Jan. 2003
234. Invited Lecture, Gas Phase Ions and Interactions, Gordon Conference, Ventura, CA, March 2003
235. Invited lecture, American Chemical Society National Meeting, Symposium Honoring Karl Christe, 2003 Inorganic Chemistry Award Winner, New Orleans, March 2003.
236. Invited Plenary Lecture NREL Workshop on Computational Science, Golden, CO, April, 2003.
237. Columbia University, Physical Chemistry Seminar, New York, NY, April, 2003 (EMSI Visiting Scholar)
238. Invited Lecture, Department of Chemistry, The University of Alabama, Tuscaloosa, AL, May, 2003.
239. Invited lecture, 35<sup>th</sup> Great Lakes ACS Regional Meeting, Symposium in honor of John Pople, Chicago, IL, June, 2003.
240. Invited Lecture, Department of Chemistry, The University of Alabama, Tuscaloosa, AL, July, 2003.
241. Invited Lecture, Symposium on New Aspects of Bonding, American Chemical Society, National Meeting, New York City, Sept. 2003

242. Invited Lecture, Symposium on Computational Toxicology, American Chemical Society, National Meeting, New York City, Sept. 2003.
243. Invited seminar, Chemistry Department, University of Nebraska-Lincoln, Nov. 2003.
244. Symposium organizer and Introductory speaker, "Controlling Chemical Transformations at the Nanoscale," AAAS Annual Meeting, Seattle, Feb., 2004.
245. Invited Lecture, "Computational Main Group Chemistry," Southeastern Theoretical Chemistry Association (SETCA), May, 2004, University of Mississippi, Oxford, MS
246. Invited Lecture, CECAM workshop on "Density Functional Theory and Hydrogen Bonding," CECAM, Lyon France, June, 2004.
247. Invited presentation, Computational Biology, JASONs study group on Computational Biology and High Performance Computing, LaJolla, CA, July, 2004.
248. Invited speaker, Symposium in Honor of H.F. Schaeffer's 60<sup>th</sup> Birthday, ACS national meeting, August, 2004.
249. Invited Speaker, Workshop on Databases for Catalysis, Purdue University, Sept., 2004.
250. Invited Speaker, PNNL Workshop on Future Directions in Catalysis, PNNL, Richland WA, Sept., 2004
251. Invited Presentation, XV Undergraduate Research Symposium, Nanotechnology, Computational Chemistry, and Computational Biology workshop, San Juan, Puerto Rico, Oct., 2004
252. Invited Seminar, Chemistry Department, Auburn University, Oct., 2004
253. Invited seminar, Chemistry Department, University of Alabama-Birmingham, Nov., 2004.
254. Invited presentation, MSCF/EMSL Workshop on Developing Needs for the NEXT MSCF Computer, PNNL, Richland WA, Dec. 2004
255. Invited lecture, 16<sup>th</sup> Winter Fluorine Conference, St. Petersburg Beach FL, Jan. 2005.
256. Invited Talk, Georgia State Students Chemistry Club, Atlanta GA, Feb., 2005.
257. Invited lecture, Computational Methods and Modeling in Fuel Chemistry Symposium, ACS National Meeting, San Diego, CA, March 2005.
258. Lead presentation, "Computational Science Drivers – Scaling in Space and Time," INEL workshop on the development of a computational science vision for INEL, INEL, Idaho Falls, ID, March, 2005.

259. Invited Panelist, "Advanced Facility Needs for Catalysis," North American Catalysis Society, Annual Meeting, Philadelphia, May, 2005.
260. Invited contribution Biogeochemical workshop, PNNL, June 2005
261. Organize symposium and lecture, Computational Chemistry, Rare Earth Research Conference, Keystone Co. June 2005
262. Invited Lecture, ORNL Workshop on Computational Chemistry and High Performance Computing, Oak Ridge National Laboratory, Oak Ridge, TN, August, 2005.
263. Invited Lecture, Structure and Function in Chemistry and Biology, Symposium Celebrating the 85<sup>th</sup> Birthday of Prof. William N. Lipscomb, Shanghai, China, August, 2005
264. Invited Lecture, Computational Chemistry at the Teraflop and Beyond Symposium, ACS National Meeting, Washington, DC, Aug. 2005
265. Invited Lecture, Chemistry of Clusters, ACS National Meeting, Washington, DC, Aug. 2005.
266. Invited presentation and breakout session organizer, DOE Workshop on the Advanced Fuel Cycle Initiative, Gaithersburg, MD, Sept., 2005.
267. Invited Lecture, XVI Undergraduate Research Symposium, Nanotechnology, Computational Chemistry, and Computational Biology Workshop, San Juan, Puerto Rico, Sept., 2005.
268. Invited Lecture, PacifiChem 2005, Symposium on Applications of Quantum Chemistry to Actinides, Honolulu, HI, Dec. 2005.
269. Invited Lecture, PacifiChem 2005, Symposium on Clusters: From the Molecular Level to Solution, Honolulu, HI, Dec. 2005.
270. Invited Lecture, Pacific Chem 2005, Symposium on Inorganic Fluorine Chemistry: From Basic Research to Applications, Honolulu, HI, Dec. 2005.
271. Invited Lecture, Wisconsin School of Pharmacy, Madison, WI, March, 2006
272. Invited Lecture, Quantitative Quantum Chemistry, Symposium in honor Thom Dunning, Santa Fe, March, 2006
273. Invited Lecture, National ACS meeting, Symposium in honor of the fluorine award winner: Boris Zemva, Atlanta, March, 2006
274. Invited Lecture, Solvay Three Day Symposium on Chemical Reactivity, Brussels, April 2006

275. Invited Tutorial on Hydrogen Storage, "Computational Chemistry for H<sub>2</sub> Storage: Theoretical Background and Applications," Materials Research Society Annual Spring Meeting, April, 2006
276. Invited Lecture, Symposium on Advances in Hydrogen Storage, Materials Research Society Annual Spring Meeting, April, 2006\
277. Invited Lecture, Theory Focus Session on Hydrogen Storage Materials, U.S. DOE Hydrogen Review Meeting, Crystal City, VA, May, 2006
278. Invited participant, presentation, and writer at the DOE BES workshop: "Basic Research for Advanced Nuclear Energy Systems," Bethesda, MD, August, 2006.
279. Invited participant, session organizer (Separations) and writer at the DOE OASCR workshop: "Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems," Washington, DC, August, 2006.
280. Invited participant, speaker, and writer, INL Workshop on "Virtual nuclear reactor center," Denver, Aug, 2006
281. Invited Lecture, Core-to-Core Program Symposium on "innovative Synthesis of Novel Main-Group Compounds and Its Applications," Tokyo, Japan, August, 2006.
282. Invited Presentation, Los Alamos/MITI Workshop on Fuel Cells and Hydrogen Storage, Santa Fe, NM, August, 2006.
283. Invited Lecture, XVII Undergraduate Research Symposium, Nanotechnology, Computational Chemistry, and Computational Biology Workshop, San Juan, Puerto Rico, Sept., 2006.
284. Invited lecture, Argonne National Laboratory, Argonne IL, Jan. 2007
285. Invited Lecture, Loker Hydrocarbon Research Institute and Department of Chemistry Symposium Honoring Professor Karl O. Christe on the Occasion of his 70th Birthday, University of Southern California, Los Angeles, CA, Jan. 2007
286. Invited Plenary Lecture, 18<sup>th</sup> Winter Fluorine Conference of the American Chemical Society, Jan. 2007.
287. Invited Lecture, Chemical Engineering Department, Mississippi State, Starksville, MS, Jan. 2007.
288. Invited Lecture: Physical Chemistry Division, Chemistry Department, University of Maryland, College Park, MD, Feb. 2007.
289. Invited lecture, Idaho National Laboratory, Idaho Falls, ID, Feb. 2007

290. Invited Lecture: Inorganic Division, Chemistry Department, Florida State University, Tallahassee, FL, March 2007.
291. 20<sup>th</sup> Coulson Lecture, Department of Chemistry, The University of Georgia, Athens GA, April, 2007.
292. Lecture, DOE Hydrogen Review, Arlington VA, May, 2007.
293. Invited Lecture, ACS National Meeting, Neil Bartlett Symposium, Fluorine Division, August, 2007, Boston Mass
294. Invited Lecture, ACS National Meeting, Computational Actinide Chemistry, Nuclear Chemistry Division, August, 2007, Boston Mass
295. Plenary lecture, Alternative energy workshop OASCR, Rockville MD Sept 2007.
296. Invited Lecture, Chemistry Department, University of North Texas, Denton, TX, Feb. 2008.
297. Invited Lecture, Chemistry Department, University of South Alabama, Mobile, AL, Feb. 2008.
298. Invited Lecture, Symposium on Computational Methods and Molecular Modeling in Fuel Chemistry, American Chemical Society (ACS), Division of Fuel Chemistry, Spring National Meeting, New Orleans, April 2008
299. Plenary lecturer, 40<sup>th</sup> Annual Southeastern Regional American Chemical Society Undergraduate Research Conference, Mississippi, College, Clinton, MS, April 2008.
300. Plenary lecture, Hydrogen Symposium 2008, Purdue University, West Lafayette, IN, April 2008.
301. Lecture, DOE Hydrogen Review, Arlington VA, June, 2008.
302. Invited lecture, SPARC workshop on the Role of Halogen Chemistry in Polar Stratospheric Ozone Depletion, Cambridge U, Cambridge, UK, June, 2008.
303. Invited presentation, Joint LANL-NEDO Workshop on Hydrogen Storage and Fuel Cells, San Diego, Sept. 2008.
304. Invited Presentation, Main Group and f-Element Chemistry Symposium, Southeastern Regional Meeting of the American Chemical Society (SERMACS), November 14, 2008, Nashville, TN
305. Invited presentation, DOE/EERE Center of Excellence in Metal Hydrides, Caltech, Pasadena, CA Dec. 2008.
306. Invited presentation, 19<sup>th</sup> Winter Fluorine Conference, St. Petersburg Beach, FL, Jan. 2009.

307. Plenary Lecture, 49<sup>th</sup> Sanibel Symposium, Feb. 2009, St. Simons Island, Georgia
308. Invited lecture, Atmospheric Chemistry Symposium, Division of Analytical Chemistry, American Chemical Society Spring National Meeting, Salt Lake City, March, 2009.
309. Invited lecture, Mississippi State University, Department of Chemistry, March, 2009, Starkville, MS
310. Lecture, DOE Hydrogen Review, Arlington VA, May, 2008.
311. Invited Lecture, ACS National Meeting, Division of Fuel Chemistry, Advances in Experimental and Computational Studies of Materials for Hydrogen Storage, Washington DC, August 2009
312. Invited Lecture, Physical Chemistry, Georgia Institute of Technology, Atlanta, GA, September 2009.
313. Invited Lecture, Chemical Engineering, Washington State University, Pullman WA, December 2010.
314. Invited Lecture & co-organizer, DOE BES Earth Sciences Council workshop: Computational Geochemistry: Predicting Properties of the Mineral-Water Interface, Annapolis, MD, January 2010.
315. Invited Lecture, Chemistry, University of Southern Mississippi, Hattiesburg, MS, February 2010
316. Invited Lecture, Center for Computational Sciences, University of Kentucky, Lexington, KY, February 2010
317. Invited Lecture, Chemistry, Washington State University, Pullman WA, March, 2010
318. Invited Lecture, ACS National Meeting, Division of Geochemistry Symposium: Predicting Molecular Properties at the Mineral-Water Interface: Challenges and Opportunities for High Performance Computing, San Francisco, March, 2010.
319. Invited lecture, Chemistry, Union University, Jackson TN, April, 2010.
320. Keynote Lecture, Goldschmidt 2010, in Section 18b, Elementary Reaction Mechanisms in Geochemistry, Knoxville TN, June, 2010.
321. Invited Lecture, University of Alabama-Birmingham, Cyberinfrastructure Day, 2010, Birmingham, AL, September, 2010.
322. Invited Lecture, ZCAM Workshop on Databases in Quantum Chemistry: Validation of methods and software and repositories of reference computational results, Zaragoza Spain, September, 2010

323. Invited lecture, CECAM Workshop on Materials for Hydrogen Storage, University College, Dublin, Ireland, October, 2010.
324. Invited Lecture, PacifiChem 2010, Symposium on Fundamental and Applied Inorganic Fluorine Chemistry and Their Impacts on Energy Conservation and the Environment, Honolulu, HI, December. 2010.
325. Invited Lecture, 20<sup>th</sup> Winter Fluorine Conference, St. Petersburg Beach, FL, Jan. 2011.
326. Invited lecture, Gordon Research Conference: Chemical Reactions at Surfaces February 6-11, 2011, Ventura CA
327. Invited Lecture, 241<sup>st</sup> ACS National Meeting, Division of Computers in Chemistry: ACS Award for Computers in Chemical and Pharmaceutical Research Award: Symposium in Honor of Thom Dunning, Anaheim, CA, March 2011.
328. Invited Lecture, 2011 SETCA Annual Meeting, Mississippi State, Starksville MS May 13-14, 2011.
329. Invited Lecture, LANSCE Summer School, Los Alamos National Lab, Los Alamos, NM, July 2011.
330. Invited Lecture, Goldschmidt 2011, 19a: Radioactivity in the Environment: Damage, Solution, and Relativistic Effects, Prague, Aug 2011.
331. Invited Lecture, 242<sup>nd</sup> ACS National Meeting, Division of Fluorine Chemistry, Symposium in Honor of Donald J. Burton: "Fluorine Chemistry the Iowa Way" Denver , Aug. 2011.
332. Invited Lecture, 242<sup>nd</sup> ACS National Meeting, Division of Environmental Chemistry, Heterogeneous Catalysis for Sustainable Energy Applications, Denver , Aug. 2011.
333. Invited Lecture, 242<sup>nd</sup> ACS National Meeting, Division of Environmental Chemistry Computational Modeling of Photo-catalysis and Photo-induced Charge Transfer Dynamics on Surfaces, Denver , Aug. 2011.
334. Invited Lecture , 242<sup>nd</sup> ACS National Meeting, Division of Fuel Chemistry, Computational Methods, Modeling, and Simulations in Fuel and Energy Technologies, Denver , Aug. 2011.
335. Invited Lecture, SIAM Conference on Parallel Processing for Scientific Computing, Savannah, GA, Feb., 2012.
336. Invited Lecture , 243<sup>rd</sup> ACS National Meeting, Division of Geochemistry, Computational Chemistry for Geochemistry, San Diego, March, 2012



337. Invited Lecture , 243<sup>rd</sup> ACS National Meeting, Division of Nuclear Chemistry and Technology, A Career in Actinide Science: Tribute to Lester Morss, San Diego, March, 2012
338. Invited Lecture, 2012 SETCA Annual Meeting, University of Georgia, Athens, GA, May 18-19, 2012.
339. Invited Lecture, Symposium on the Chemistry and Physics of the Heavy Elements, Santa Fe, NM, June 20-22, 2012.
340. Invited Lecture, Arkema, King of Prussia, PA, Aug. 2012
341. Invited Lecture, 9th Mississippi State - UAB Conference on Differential Equations and Computational Simulations, Mississippi State University, Oct. 4-6, 2012.
342. Invited Lecture, 21<sup>st</sup> Winter Fluorine Conference, St. Petersburg Beach, FL, Jan. 2013
343. Invited Lecture, Inaugural SEC Symposium, Renewable Energy, Atlanta GA, Feb., 2013
344. Tennessee Tech, Department of Chemistry, seminar, Cookeville, TN, Feb. 2013
345. Invited Lecture, SIAM Conference on Parallel Processing for Scientific Computing, Boston MA, Feb. 2013.
346. Invited Lecture , Division of Energy and Fuels, Symposium: Bioenergy and Biofuels, 245<sup>th</sup> ACS National Meeting & Exposition, New Orleans, LA, April, 2013.
347. Invited Lecture, Division of Fluorine Chemistry, ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Iwao Ojima, 245<sup>th</sup> ACS National Meeting & Exposition, New Orleans, LA, April, 2013
348. Invited Lecture, Division of Catalysis Science and Technology, Symposium on Catalysis by Materials with Well-Defined Structures, 245<sup>th</sup> ACS National Meeting & Exposition, New Orleans, LA, April, 2013.
349. Invited Lecture, Division of Geochemistry, Symposium on Atomistic Computational Geochemistry: Atomic-Level Processes with Macroscopic Implications, 245<sup>th</sup> ACS National Meeting & Exposition, New Orleans, LA, April, 2013.
350. Invited Lecture, Advanced Photon Source (APS) User Meeting, Workshop on Combining Experiments and Theory in f-Element Research, Argonne National Laboratory, Argonne IL May 6-9, 2013
351. Invited Lecture, 2013 SETCA Annual Meeting, Auburn University, May 10-11, 2013.
352. Invited Lecture, Session on “Theoretical and Experimental Approaches to Geochemical Reactions, Including Solvation, Complexation, Adsorption, and Redox,” 2013 Goldschmidt Conference, Florence, Italy, August 2013.

353. Invited Lecture, Division of Environmental Chemistry, Symposium on Heterogeneous Catalysis for Environmental and Energy Applications, 246<sup>th</sup> ACS National Meeting, Indianapolis, In, Sept. 2013
354. Invited Lecture, Division of Fluorine Chemistry, Symposium on Current Topics in Industrial Fluorine Chemistry, 247<sup>th</sup> ACS National Meeting, Dallas, TX, March 2014.
355. Invited Lecture, Division of Nuclear Chemistry, Symposium on Thermodynamics, Reactivity, and Spectroscopy of the Heavy Elements, 247<sup>th</sup> ACS National Meeting, Dallas, TX, March 2014.
356. Invited lecture DOE PI Catalysis meeting July 2014
357. Keynote Lecture, ORNL User meeting July 2014
358. Invited Lecture, Division of Fluorine Chemistry, Exploring the Frontiers of Fundamental and Applied Fluorine Chemistry: Symposium in Honor of Gary J. Schrobilgen, 248<sup>th</sup> ACS National Meeting, San Francisco, August 2014.
359. Invited Lecture, Division of Environmental Chemistry, Symposium on Heterogeneous Catalysis for Environmental and Energy Applications, 248<sup>th</sup> ACS National Meeting, San Francisco, August 2014
360. Invited lecture, International Conference on Theoretical and High Performance Computational Chemistry-2014, Beijing China, Sept. 2014.
361. Invited Lecture, 22<sup>nd</sup> Winter Fluorine Conference, St. Petersburg Beach, FL, Jan. 2015.
362. Invited Lecture, Division of Fluorine Chemistry, Fluorine Award Symposium, 249<sup>th</sup> ACS National Meeting, Denver, March 2015
363. Invited Lecture, Division of Fluorine Chemistry, Iodine Award Symposium, 249<sup>th</sup> ACS National Meeting, Denver, March 2015
364. Invited Lecture, Division of Nuclear Chemistry, Convergence of Theory and Experiment Symposium, 249<sup>th</sup> ACS National Meeting, Denver, March 2015
365. Invited Lecture, Rimes Lecture, Springhill College, Mobile AL, April, 2015
366. Invited Lecture, 2015 SETCA Annual Meeting, University of Central Florida, May 14-16, 2015.
367. Invited Lecture, Division of Computational Chemistry, 250<sup>th</sup> ACS National Meeting, Boston, August 2015.
368. Invited Plenary Lecture, DOE High Performance Computing Operational Review (HPCOR) on Scientific Software Architecture for Portability and Performance, Gaithersburg. MD, Sept. 2015.

369. Invited lecture, Current Trends and Interconnectivities among Fundamental and Applied Inorganic Fluorine Chemistry, Pacificchem Honolulu HI, Dec. 2015
370. Invited lecture, Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications, Pacificchem Honolulu HI, Dec. 2015
371. Invited lecture, Theory of Main Group Chemistry Beyond First Row, Pacificchem Honolulu HI, Dec. 2015
372. Invited lecture, 251<sup>st</sup> ACS National Meeting, Division of Nuclear Chemistry, San Diego, CA, March, 2016
373. Invited lecture, 251<sup>st</sup> ACS National Meeting, Division of Nuclear Chemistry, San Diego, CA, March, 2016
374. Invited lecture, 251<sup>st</sup> ACS National Meeting, Division of Nuclear Chemistry, San Diego, CA, March, 2016.
375. Invited Lecture, Berlin, Humboldt University, May 2016
376. Invited Lecture, Berlin, Freie Universitat-Berlin, May 2016