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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The University of Alabama
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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, 2010-2016

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, Fellow, 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, 20th 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

2016, 5th Annual Burris Cunningham Actinide Science Seminar, Lawrence Berkeley National Laboratory

2017 Listed as a top author in the *Journal of Physical Chemistry A*

2018 Blackmon-Moody Award, The University of Alabama

2019, The University of Alabama President's Faculty Research Award, Senior Level, STEM

Publications: Total = 865 + patents

h-index = 94, >40,000 citations

Peer-reviewed, published: 765 (400 at UA)

Book Chapters/Books: 54

Edited 6 volumes of *Annual Reports in Computational Chemistry* (all at UA)

Proceedings Contributions and extended preprints: 32 (8 at UA)

Book reviews and Prefaces: 5 (2 at UA)

Corporate journals: 3

Patents: 3 + 1 provisional (provisional at UA)

Invited Presentations: 400 (157 at UA)

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, 2nd Semester Graduate Quantum Mechanics, Winter/Spring, University of Pennsylvannia.

2004, 2005 (Fall), Introductory Chemistry II (CH102)

2004-present, Computer Based Honors Program, now Randall research Scholars Program

2006 (Spring), Graduate Statistical Mechanics, Thermodynamics, and Kinetics CH541

2006-2012 (Fall), Honors Introductory Chemistry I CH117

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

2013-2017 (Fall) Physical Chemistry (Quantum Mechanics) for ACS undergraduate majors and chemistry graduate students CH341

2017 (Spring) Majors Physical Chemistry Laboratory CH348

2018-2019 (Fall) Honors Introductory Chemistry I, CH117; Physical Chemistry for BS Chemistry Degree, CH340

2020 (Fall) CH519 Introductory Physical and Analytical Chemistry for Gradaute Students

Adjunct Positions

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

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 20th anniversary of the Chemistry Department.

Editor

Annual Reports in Computational Chemistry, Vol. 11 (2015), Vol. 12 (2016), and Vol. 13 (2017).

Editorial Boards

1988 –,present, *The International Journal of High Performance Computing Applications*

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

2011-2016, Editorial Advisory Board *The Journal of Physical Chemistry*

2012-present, *Journal of Fluorine Chemistry*

2014-present, *Computational and Theoretical Chemistry*

2020-present, *High Energy Chemistry*

American Chemical Society Service

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

1998, Chair, ACS Division of Fluorine Chemistry

2013-present, Councilor, ACS Division of Fluorine Chemistry

2013-present, Executive Committee, ACS Division of Fluorine Chemistry

2016-2021, ACS Joint Board-Council Committee on Publications (member), 2014-2015, Associate member)

Society memberships

American Chemical Society (ACS)

American Physical Society (APS)

American Association for the Advancement of Science (AAAS)

Association for Computing Machinery (ACM)

Society for Mathemtical Biology

Geochemical Society

Society for Industrial and Applied Mathematics (SIAM)

Selected External Committees and Workshops

1987 Raveché Panel that wrote "A National Computing Initiative"

1988 Planning Committee: 2nd International Conferences on Supercomputing

1989 Planning Committee: 3rd 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: 4th 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

1995-1997 Review Panel for the Chemistry Division of NIST

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

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 234th American Chemical Society National Meeting, Division of Fuel Chemistry, "Hydrogen Storage and Fuel Cell Technology", Boston

2008 Organizer of Southeast Theoretical Chemistry Association (SETCA) annual meeting, The University of Alabama

2008 Symposium Organizer at the 235th American Chemical Society National Meeting, Division of Fuel Chemistry, "Computational Methods and Modeling in Fuel Chemistry", New Orleans.

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, 20th Winter Fluorine Conference, St. Petersburg Beach, FL

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

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

2014-2016, OLCF (Oak Ridge Leadership Computing Facility) User Executive Board, Oak Ridge National Laboratory

2015 Co-Organizer, 22nd 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, 249th 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, 249th ACS National Meeting, Denver, March.

2016 Co-Organizer, Symposium: Geochemistry of the Subsurface: CO_2 Sequestration, Unconventional Oil & Gas Extraction, Geothermal Reservoirs & Radioactive Waste Disposal, Division of Geochemistry, 252nd ACS National Meeting, Philadelphia, August

2017, Basic Research Needs Workshop: Molten Salt Reactors, Office of Nuclear Energy, Department of Energy, ORNL, April

2018, Organizer, ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Erhard Kemnitz, Division of Fluorine Chemistry, 255th ACS National Meeting, New Orleans, March

PhD Students (U. MN):

Robert A. Eades *Theoretical Studies of the Abstraction Reactions of the Hydrogen Atom with halogen and Interhalogen Molecules: H + F_2, H + Cl_2, H + Br_2, H + ClF, H + BrF, and H + BrCl*, (PhD, 1983), IBM

Mark Ellenberger *Dynamics of Chemical Reactions: Ion Cyclotron Resonance and Crossed Molecular Beam Studies* (PhD, 1983) Independent Non-Profit Organization Management Professional, St. Paul, MN

Steven C. Richtsmeier *The Structure of Small metal Clusters and Molecular Beam Studies of Weakly Bonded Systems*, (PhD, 1983) Principal Scientist, Spectral Sciences, Inc.

Robert Glinski *Chemiluminescence Studies of the Reactions of Ozone with Small Molecules*, (PhD, 1983), Prof., Chemistry, Tennessee Tech

David Weil *Studies of Organic Ion-Molecule Reactions by Ion Cyclotron Resonance Spectroscopy*, (PhD, 1984) Applications Scientist at Agilent Technologies

PhD students (UA):

Keith Gutowski *Computational Thermodynamic Studies of the Formation and Stability of Ionic Liquids and Actinide-Ligand Complexes* (PhD, 12/2006), BASF

Raluca Craciun *Computational Studies of Transition Metal Catalyst*s, (PhD, 5/2010), Wheaton College

Daniel Grant *Structure Heats of Formation, and Bond Dissociation Energies of Group IIIA–Group IVA–Group VA Molecules for Chemical Hydrogen Storage Systems* (PhD, 8/2010), Rustoleum

Monica Vasiliu *Computational Thermodynamic Studies of Alkali and Alkaline Earth Compounds, Olefin Metathesis Catalysts and Borane-Azoles for Chemical Hydrogen Storage Materials* (PhD, 8/2010), Research Scientist, The University of Alabama

Tsang-Hsui Wang *The Computational Studies on the Chemistry of Titanium Dioxide Nanoparticles* (PhD, 8/2010) Kimoto Tech Inc., deceased 2019.

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

Amanda Stott *Computational Studies of Solid State Materials for Practical Applications* (PhD, 5/2012) American Family Insurance, Atlanta

Mingyang Chen *Development and Apllications in Computaitonal Chemistry for Inorganic Catalysis* (PhD, 8/2013) Associate Prof., University of Science and Technology Beijing, (Center for Green Innovation, School of Materials Science and Engineering

Virgil Jackson, *Reliable Predictions of the Properties of Actinide Complexes*, (PhD, 12/2013) Assistant Prof. Spring Hill College

Zongtang Fang *Computational Studies of the Catalytic Reactions of Group IVB and VIB Transition Metal Oxide Clusters*(PhD, 5/2014), Idaho National Laboratory

Ted Garner *Computational Studies of Atmospheric Chemical Processes, Flexible Catalysts and, of New Materials for Chemical Hydrogen Storage* (PhD, 8/2014), Patent Lawyer, AdamsIP, LLC, Mobile

Tanya Mikulas *Electronic Strucutre Investigation of Titanium Oxide Nanoclusters, Boron-Nitrogen Heterocycles, and Reaction Products of Lanthanides with Oxygen Diflouride and Lanthanides with Water* (PhD, 5/2015), Tesla

Michele Stover *Computational Studies of the Fundamental Thermodynamic Properties of Amino Acids and Small Peptides* (PhD, 8/2015), Baylor University

Shengjie Zhang *Computational Study of the Fundamental Thermodynamic Properties of Iridium and Osmium Clusters* (PhD, 8/2017), Postdoc UA, Postdoc, LSU

Luis Flores *Computational Studies of Lewis Acidic Gas Adsorption to Transtion Metal Oxide Nanoclusters and Metal Orgnaic Frameworks* (PhD, 8/2017) U.S. EPA, Chicago

Johnny Lightcap *Observation and Elecronic Properties of Reactive Intermediates from Measurement and Electronic Structure Calculations* (PhD, 5/2018) Mitchell Cancer Institute, Mobile

Ashley McNeil *Computational Thermodynamics of gas and solution phase anions* (PhD, 8/2020) Springfield College (MA)

Matthew Confer *Experimental and Computational Studies of Materials Decomposition* (PhD, 12/2020) postdoc UA

Zachary Lee (5th year)

Randy Persaud (5th year)

Marcos Mason (4th year)

Yiqin Hu (3rd year)

Caitlin Hanson (2nd year)

Eddy Lontchi (2nd 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, Univeristy 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, 2010-2016, Staff Scientist UA (2016-current)

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

Kanchana (Sahan) Thanthiriwatte 2011-4/2017

Mariano Mendez Chavez, 2013-5/2016

Mingyang Chen, 2013 (see above)

Virgil Jackson, 2014-2015 (see above)

Zongtang Fang, 2014-10/2017 (see above)

Shengjie Zhang, 8/2017-8/2018 (see above)

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 (>100 total)

Current (as of 04/2020)

Maddie Vegrzyn, freshman, 0.5 yr., computational biomass chemistry

Barbara (Georgie) Fickling, freshman, 0.5 yr., computational MOF acid gas chemistry

William McCloud, junior, 0.5 yr., development of hypersonic fuel

Maryam Salome, sophomore, 0.5 yr., computational peptide chemistry

Skyler Lambert, junior, 2.5 yr., computational peptide chemistry, Randall Research Award, 2020

David Furniss, junior, 1.0 yr, computational peptide chemistry

Nick Parsa, 1.5 yr, junior, computational peptide chemistry, Randall Research Award, 2020

Dom Schiano, senior, 0.5 yr, computational homogeneous catalysis chemistry

Kelsey Hornbuckle, junior, 1.0 yr, computational fluorocarbon chemistry

Alyssa Caccamo, senior, 0.5 yr, computational actinide chemistry

Justin Adam, junior, 1.5 yr., computational peptide chemistry, Randall Research Award, 2020

Hannah Slater, junior, Randall Research Scholar, 2.0 year, computational heavy element chemistry and drug design, Randall Research Award, 2020

Brianna Pniak, sophomore, 1.5 yr, computational chemistry of transition metal oxyfluorides

Former

Chris Hannigan, senior, 1.0 year, computational peptide chemistry

Nicole Desotel, junior, 0.5 yr, hydricity

Ladarius Quinn, senior, 1.5 yr., metal clusters sincluding actinides

Carris Smith, senior, 3.0 yr., design of separations systems for nuclear waste, Randall Research Award 2019

Nick Benedetto, sophomore, 0.5 yr, Emerging Scholars Program, Peptide molecular dynamics

Jack O'Donohue, freshman, 0.5 yr, Emerging Scholars Program, metal clusters and computational infrastructure

Jake Patterson, sophomore, 0.5 year, experimental fuel chemistry

Lauren Tatina, sophomore, 0.5 year, computational heavy element chemistry

Julia Kessel, senior, 1.5 yr, computational heavy element chemistry

Donna Xia, senior, CBHP, 2.5 yr, computational heavy element chemistry, Randall Research Award 2017, 2018, 2019, Pettus Randall Scholarship, 2018, Goldwater Scholar, 2018, Catherine J. Randall Award, 2019.

Amber Gomez senior, 1.5 yr, computational heavy element chemistry, Randall Research Award 2019

Ashley Eberly, senior, 1.0 yr., computational heavy element chemistry, Randall Research Award 2019

Hope Burnham, senior, 3 yrs., development of hypersonic fuel, Randall Research Award 2019, 1st place in oral presentation at UA URSCA

Trent Stein, Shelton State, 2 years + 2 summers, Richland High School, Richland WA

Elizabeth Hartmann, sophomore, 0.5 yr., computational peptide chemistry

Elliot Lackner, senior, 2 yr., metal cluster chemistry

Adam Hartley, REU Summer 2017, heavy element chemistry

Cristena Rogers, sophomore, 1.0 yr, computational anion peptide charging chemistry

Matthew Fisher, sophomore, 0.5 yr, computational catalysis

Tyler Crawford, junior, 0.5 yr, computational anion peptide charging chemistry

Michael Outlaw, junior, CBHP, 2.0 yr, computational studies of catalysis

Hayden Arnold, senior, CBHP, 3.0 yr, computational studies of actinides, Randall Research Award, 3 years

Shuwen Yue, CBHP, 4.0 year, Benchmarking catalytic reactions, Computational studies of models of the Schrock and Grubbs catalysts, Randall Research Award – 3 years

Sean Miller, Emerging Scholar, 3.5 year, Chemistry research, 1 year, Computational studies of phosphorylated amino acids, 2015 Randall Research Award

Julia Murphy, 2.0 yr, Chemistry research, Carbonate formation from the reactions of CO_2 with transition metal oxides.

Jonathan Belcher, 1.0 yr, Emerging Scholar, The Ethanol Condensation Reaction on M_2O_4 (M=Ti, Zr, Hf) Nanoclusters

Will Jackson, 1.5 yr, Chemistry research, Gas-Phase Acidities of Acid-Substituted Dipeptides

Caroline Bloodworth, CBHP, 1.0 yr, computational studies of fluorocarbon thermochemistry

William Layfield, CBHP, 1.5 yr, computational studies of actinides

Emma Clements, CBHP, 1.0 yr, computational studies of actinides

Laura Holland, 1.0 yr, computational studies of peptide chemistry

Blake Copeland, 1.0 yrChemistry research, Nitrate formation from the reactions of NO_2 with transition metal oxides

Jacob Owen, 1.0 yr, Chemistry research, Computational biochemistry, peptide acidities

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

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

Steven Spellmon, Emerging Scholar, 1.5 year, Chemistry research, 1 year, Converting CO_2 to MeOH using Frustrated Lewis Pairs

Patrick Zetterholm, Emerging Scholar, 0.5 year, Computational Studies of Trimethylene Glycol Conversion on a $(WO_3)_3$ 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_2 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 oxolation and olation 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 3rd 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_2 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_2 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); 2nd 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; 3rd 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 2nd 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 3rd 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.

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
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
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
4. "Search for the $Br_2 + Cl_2$ Exchange Reaction," D. A. Dixon, D. L. King, and D. R. Herschbach, *Faraday Discuss. Chem. Soc.*, **1973**, *55*, 375-376. DOI: 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
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
7. "Localized Orbitals in Large Boron Hydrides. $B_{16}H_{20}$ 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
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
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"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)

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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, Compuational 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, Pacifichem Honolulu HI, Dec. 1989

78. Invited lecture, Pacifichem 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, 15th International Symposium on Fluorine Chemistry in Vancouver, BC, Aug. 1997.

177. Invited Lecture, 5th 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, 6th 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, 13th Canadian Symposium on Theoretical Chemistry, Vancouver, BC, Aug. 1998.

188. Invited Lecture, ACS National meeting, Schrobilgen Fluorine Award Symposium Aug. 1998.

189. Invited lecture, 15th 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, 2nd 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 21st 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, 15th 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, 35th 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 60th 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, 16th 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 85th 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_2 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^{th} 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. 20th 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, 40th 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, 19th Winter Fluorine Conference, St. Petersburg Beach, FL, Jan. 2009.

307. Plenary Lecture, 49th 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, 20th 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, 241st 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, 242nd 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, 242nd ACS National Meeting, Division of Environmental Chemistry, Heterogeneous Catalysis for Sustainable Energy Applications, Denver , Aug. 2011.

333. Invited Lecture, 242nd 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 , 242nd 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 , 243rd ACS National Meeting, Division of Geochemistry, Computational Chemistry for Geochemistry, San Diego, March, 2012

337. Invited Lecture , 243rd 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, 21st 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, 245th 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, 245th 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, 245th 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, 245th 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, 246th ACS National Meeting, Indianapolis, In, Sept. 2013

354. Invited Lecture, Division of Fluorine Chemistry, Symposium on Current Topics in Industrial Fluorine Chemistry, 247th ACS National Meeting, Dallas, TX, March 2014.

355. Invited Lecture, Division of Nuclear Chemistry, Symposium on Thermodynamics, Reactivity, and Spectroscopy of the Heavy Elements, 247th 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, 248th ACS National Meeting, San Francisco, August 2014.

359. Invited Lecture, Division of Environmental Chemistry, Symposium on Heterogeneous Catalysis for Environmental and Energy Applications, 248th 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, 22nd Winter Fluorine Conference, St. Petersburg Beach, FL, Jan. 2015.

362. Invited Lecture, Division of Fluorine Chemistry, Fluorine Award Symposium, 249th ACS National Meeting, Denver, March 2015

363. Invited Lecture, Division of Fluorine Chemistry, Iodine Award Symposium, 249th ACS National Meeting, Denver, March 2015

364. Invited Lecture, Division of Nuclear Chemistry, Convergence of Theory and Experiment Symposium, 249th 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, 250th 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, Pacifichem Honolulu HI, Dec. 2015

370. Invited lecture, Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications, Pacifichem Honolulu HI, Dec. 2015

371. Invited lecture, Theory of Main Group Chemistry Beyond First Row, Pacifichem Honolulu HI, Dec. 2015

372. Invited lecture, 251st ACS National Meeting, Division of Nuclear Chemistry, San Diego, CA, March, 2016

373. Invited lecture, 251st ACS National Meeting, Division of Nuclear Chemistry, San Diego, CA, March, 2016

374. Invited lecture, 251st 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

377. Keynote Lecture, 252nd ACS National Meeting, Division of Energy and Fuels, Degradation of Materials for Energy & Fuel Production Symposium,ACS Philadelphia, August, 2016

378. 5th Annual Burris Cunningham Actinide Science Seminar, Lawrence Berkeley National Laboratory, Nov. 2016

379. Keynote Lecture, 23rd Winter Fluorine Conference, Clearwater Beach, FL, January, 2017

380. Invited lecture, 253rd ACS National Meeting, Division of Nuclear Chemistry, Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark, San Francisco, April, 2017.

381. Invited lecture, 253rd ACS National Meeting, Division of Nuclear Chemistry, Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten, San Francisco, April, 2017.

382. Invited lecture, 253rd ACS National Meeting, Division of Catalysis Science and Technology, Amorphous Catalytic Materials, San Francisco, April, 2017

383. Invited lecture, 253rd ACS National Meeting, Division of Energy and Fuels, Computations for CO_2 Capture, Conversion & Sequestration, San Francisco, April, 2017

384. Invited lecture, 2017 SETCA Annual Meeting, University of Mississippi, Oxford, MS, May 2017.

385. Invited Lecture, SERMACS, Organofluorine Chemistry Symposium, Charlotte, NC, Nov. 2017

386. Invited Lecture, University of Southern California, Inorganic Chemistry, Los Angeles, Nov. 2017

387. Invited Lecture, Auburn University, Jan, 2018

388. Invited Lecture, University of Georgia, CCQC, Jan 2018

389. Invited Lecture, University of Georgia, Physical Chemistry Division, Jan 2018.

390. Invited Lecture, 255th ACS National Meeting, Division of Fluorine Chemistry, ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Erhard Kemnitz, New Orleans, April, 2018

391. Invited Lecture, 255th ACS National Meeting, Division of Nuclear Chemistry, Actinide Complexes & Nanoclusters, New Orleans, April, 2018

392. Invited Keynote Lecture, International Fluorine Symposium, Oxford, England, July 2018.

393. Invited Plenary Lecture, 24th Winter Fluorine Conference, Clearwater Beach, FL, Jan. 2019.

394. Invited Lecture, Gas Phase Clusters- Experiment and Theory in Concert, Division of Chemical Physics, APS National Meeting, Boston MA, March 2019

395. Invited Lecture, 257th ACS National Meeting, Division of Catalysis Science and Technology, Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy and the Environment, Orlando FL, April, 2019.

396. Invited Lecture, Advanced Photon Source Users Meeting, Separations Workshop, Argonne National Laboratory, May 2019

397. Invited Lecture, 258th ACS National Meeting, Division of Nuclear Chemistry, Computational Methods for Lanthanides and Actinides, San Diego, CA, August 2019.

398. Invited Lecture, 258th ACS National Meeting, Computers in Chemistry Division, Exploring Transition Metal Chemistry and Spectroscopy with Quantum Chemistry, San Diego, CA, August 2019.

399. Invited Lecture, 258th ACS National Meeting, Computers in Chemistry Division, Advances in Multiscale Computational Modeling of Biomass Conversion Processes, San Diego, CA, August 2019.

400. Invited Lecture, Department of Chemistry, University of Memphis, Memphis, TN, November, 2019

Grants funded at The University of Alabama Since 1/1/2014

Funding Source: DOE – Office of Environmental Management Science Program (EMSP)
Title: Chemical Speciation of Strontium, Americium, and Curium in High Level Waste: Predictive Modeling of Phase Partitioning During Tank Processing
PI: A.R. Felmy (PNNL)
Project Period: 10/01/2003 - 09/30/2006
Annual Funding: $ 235K, $20K per year to DAD 0 month

Funding Source: Department of Energy (DOE) – Office of Science, Basic Energy Science (OBES)
Title: Size and Shape Effects on Surface Charging and Energetics of Goethite Nanoparticles
PI: A. Felmy (PNNL)
Project Period: 10/1/2003 – 9/30/2006
Annual Funding: $150K, $30K per year to DAD

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Early Transition Metal Oxides as Catalysts: Crossing Scales from Clusters to Single Crystals to Functioning Materials
PI: D.A. Dixon (original), current, C. Peden (PNNL)
Project Period: 10/1/2003 – 9/30/2006
Annual Funding: 2,100,000. $136 K to D.A. Dixon

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Molecular Basis for Microbial Adhesion and Geochemical Surface Reactions: A Study Across Scales
PI: T.P. Straatsma (PNNL), D.A. Dixon (co-PI)
Project Period: 1/1/2006 – 9/30/2008
Annual Funding: $45 K to D.A. Dixon

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Early Transition Metal Oxides as Catalysts: Crossing Scales from Clusters to Single Crystals to Functioning Materials
PI: C. Peden (PNNL), D.A. Dixon (co-PI)
Project Period: 10/1/2006 – 9/30/2009
Annual Funding: 2,100,000, $136 K to D.A. Dixon

Funding Source: U. S. Civilian Research & Development Foundation (CRDF)
Title: Investigation of the Stability Origin of Long-lived in Liquid Perfluorocarbon Radicals and Searching the Ways of their Application
PI: DA Dixon
Project Period: 8/15/2006 – 8/15/2008
Annual Funding: $85K

Funding Source: Department of Energy (DOE) – Office of Science, Basic Energy Science (OBES)

Title: The Impact of Carbonate on Surface Protonation, Electron Transfer and Crystallization Reactions in Iron Oxide Nanoparticles and Colloids
PI: J.R. Rustad (UC-Davis), D.A. Dixon (co-PI)
Project Period: 10/1/2006 – 9/30/2009
Annual Funding: $225K, $60K per year to D.A. Dixon

Funding Source: Sentient Corporation for the United States Army Space and Missile Defense Command (USASMDC) – Redstone Arsenal
Title: The Development of Chemical Hydrogen Release Materials for the Army Hypersonic Technologies Program Through the Use of Computational Chemistry
PI: D.A. Dixon
Project Period: 2/1/2008 – 12/31/2008
Annual Funding: $100K

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Molecular Basis for Microbial Adhesion and Geochemical Surface Reactions: A Study Across Scales
PI: T.P. Straatsma (PNNL), D.A. Dixon (co-PI)
Project Period: 10/01/2008 – 9/30/2009
Annual Funding: $50 K to D.A. Dixon

Funding Source: DOE Energy Efficiency/Renewable Energy (EE/RE)
Title: Chemical Hydrogen Storage Center
PI: William Tumas (LANL), D.A. Dixon (co-PI)
Project Period: 2/1/2005 – 3/31/2010
Annual Funding: ~$5,000,000. $300K to UA

Funding Source: Sentient Corporation for the United States Army Space and Missile Defense Command (USASMDC) – Redstone Arsenal
Title: The Development of Chemical Hydrogen Release Materials for the Army Hypersonic Technologies Program Through the Use of Computational Chemistry
PI: D.A. Dixon
Project Period: 2/1/2009 – 12/31/2009 (extension to 05/15/2010)
Annual Funding: $100K

Funding Source: Sentient Corporation for the United States Army Space and Missile Defense Command (USASMDC) – Redstone Arsenal
Title: SBIR: High Density H2 Phase Changing Missile Fuel
PI: DA Dixon (at UA), Project PI: Kent Key, Sentient COrp
Project Period: 03/01/2011 – 02/28/2012
Total Funding: $40,000

Funding Source: Department of Energy, EERE
Project Title: Hydrogen Storage by Novel CBN Heterocycle Materials
PI: S.-Y. Liu (U. Oregon), David Dixon (co-PI)
Project Period: 04/01/2010-03/31/2011

Annual funding: $25K to D.A. Dixon (0.08 FTE summer, 2 graduate students, 1 postdoctoral fellow)

Funding Source: National Science Foundation
Title: NIRT: Active Nanoparticles in Nanostructured Materials Enabling Advances in Renewable Energy and Environmental Remediation
PI: DA Dixon
Project Period: 8/15/2006 – 8/15/2010
Annual Funding: $275K

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Supported Molecular Catalysts: Synthesis, Structure, and Catalytic Cycles
PI: H. Haw (USC), D.A. Dixon (co-PI)
Project Period: 1/1/2008 – 12/14/2010
Annual Funding: $82 K to D.A. Dixon

Funding Source: Department of Energy (DOE) – Office of Science, Advanced Scientific Computing Research
Title: The Computational Chemistry End Station (ChemES)
PI: Robert J. Harrison (ORNL, UTenn), D.A. Dixon (co-PI)
Project Period: 12/15/2007 – 12/31/2009 (extension to 12/31/2010)
Annual funding: $2M for 2 years, $100K to DAD/yr

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Molecular Basis for Microbial Adhesion and Geochemical Surface Reactions: A Study Across Scales
PI: D.A. Dixon (PI)
Project Period: 01/01/2009 – 12/31/2011
Annual Funding: $50 K to D.A. Dixon

Funding Source: NSF
Title: Mass Spectrometry and Computational Studies of Deprotonated Peptides and Amino Acid Amides
PI: C. Cassady (UA), D.A. Dixon (co-PI)
Project Period: 01/01/2009 – 12/31/2011
Annual Funding: $140 K (1 graduate student support)

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Early Transition Metal Oxides as Catalysts: Crossing Scales from Clusters to Single Crystals to Functioning Materials
PI: C. Peden (PNNL), D.A. Dixon (co-PI)
Project Period: 10/1/2009 – 9/30/2012
Annual Funding: $155 K to D.A. Dixon

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)

Title: Dispersed Metal Cluster Catalysts by Design: Synthesis, Characterization, Structure, and Performance
PI: B. Gates (UC-Davis), D.A. Dixon (co-PI)
Project Period: 8/1/2011 – 9/30/2013
Annual Funding: $77 K to D.A. Dixon

Funding Source: NSF
Title: Mass Spectrometry and Computational Studies of Deprotonated Peptides and Amino Acid Amides
PI: C. Cassady (UA), D.A. Dixon (co-PI)
Project Period: 01/01/2009 – 12/31/2011
Annual Funding: $140 K

Funding Source: Department of Energy, Office of Basic Energy Sciences
Project Title: SISGR: Mineral Transformations in Supercritical CO_2-Dominated Fluids: Impact on Caprock Integrity
PI: Andrew Felmy (PNNL), David Dixon (co-PI)
Project Period: 10/01/2009 – 9/30/2012
Annual Funding: $65K to D.A. Dixon (0.05 FTE summer, 1 postdoctoral fellow)

Funding Source: Department of Energy, Office of Basic Energy Sciences
Project Title: SISGR: Understanding Actinide Aggregation
PI: Lynne Soderholm (ANL), David Dixon (co-PI)
Project Period: 10/01/2009 – 09/30/2012
Annual funding: $120K to D.A. Dixon (0.08 FTE summer, 2 graduate students, 1 postdoctoral fellow)

Funding Source: Department of Energy, Nuclear Energy University Programs – Infrastructure Support Program
Project Title: Infrastructure for Solid State, Solution, and Theoretical Actinide Chemistry for the Introduction into Radiochemistry Curriculum at The University of Alabama
PI: Robin Rogers, David Dixon (co-PI)
Project Period: 10/01/2009 – 09/30/2012
Annual funding: $185,342 for instrumentation

Funding Source: Howard Hughes Medical Institute
Project Title: 2010 Howard Hughes Medical Institutue Precollege and Undergraduate Science Education Program to The University of Alabama
PI: Martha Powell (Biology, UA), David Dixon (co-PI)
Project Period: 09/01/2010 – 08/31/2014
Total funding: $1,500,000. Funds to DAD will be used to update the Honors Freshman Chemistry Laboratory and to continue to develop a Freshman Learning Community seminar in Energy and the Environment

Funding Source: Sentient Corporation for the United States Army Space and Missile Defense Command (USASMDC) – Redstone Arsenal

Title: High Density Phase Changing Missile Fuel: SBIR II
PI: D.A. Dixon
Project Period: 6/1/2012 – 5/31/2014
Annual Funding: $167K

Funding Source: Argonne National Laboratory
Project Title: *Support of Argonne National Laboratory Strategic Initiatives*
PI: David Dixon (PI)
Project Period: 10/01/2011 – 9/30/2012
Annual funding: $120K

Funding Source: NSF
Project Title: *Experimental and Theoretical Study of Ligand Steric Effects in Homogeneous Catalysis*
PI: K. Shaughnessy (PI), David Dixon (co-PI)
Project Period: 09/01/2011 – 8/31/2014
Annual funding: $50K

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Chemical Transformations at Complex Interfaces
PI: J. Lercher (PNNL), D.A. Dixon (co-PI)
Project Period: 10/1/2012-9/30/2015
Annual Funding: $120 K to D.A. Dixon

Funding Source: DOE – Office of Science, Basic Energy Science (OBES)
Title: Dispersed Metal Cluster Catalysts by Design: Synthesis, Characterization, Structure, and Performance
PI: B. Gates (UC-Davis), D.A. Dixon (co-PI)
Project Period: : 8/1/2011 – 3/31/2015
Annual Funding: $77 K to D.A. Dixon

Funding Source: NSF
Title: Mass Spectrometry and Computational Studies of Deprotonated Peptides and Amino Acid Amides
PI: C. Cassady (UA), D.A. Dixon (co-PI)
Project Period: 01/01/2013 – 5/31/2016
Annual Funding: $140 K

Funding Source: Department of Energy, Office of Basic Energy Sciences
Project Title: Molecular Mechanisms of Interfacial Reactivity in Near Surface and Extreme Geochemical Environments
PI: Andrew Felmy (PNNL), David Dixon (co-PI)
Project Period: 10/01/2012 – 9/30/2015
Annual Funding: $65K to D.A. Dixon (0.05 FTE summer, 1 postdoctoral fellow)

Funding Source: Department of Energy, Office of Basic Energy Sciences

Project Title: Understanding Actinide Aggregation
PI: Lynne Soderholm (ANL), David Dixon (co-PI)
Project Period: 10/01/2012 – 09/30/2015
Annual funding: $120K to D.A. Dixon (0.08 FTE summer, 2 graduate students, 1 postdoctoral fellow)

Funding Source: Department of Energy, EERE
Project Title: Novel Carbon (C) – Boron (B) – Nitrogen (N) – Containing H_2 Storage Materials
PI: S.-Y. Liu (Boston College), David Dixon (co-PI)
Project Period: 1/1/2012 – 9/30/2015
Annual funding: $340,000, $67K to D.A. Dixon

Funding Source: Sentient Corporation for the United States Army Space and Missile Defense Command (USASMDC) – Redstone Arsenal
Title: High Density Phase Changing Missile Fuel: SBIR II
PI: D.A. Dixon
Project Period: 6/1/2012 – 5/31/2015
Annual Funding: $167K (2 years, 1 year no cost extension)

Funding Source: Argonne National Laboratory
Project Title: *Support of Argonne National Laboratory Strategic Initiatives*
PI: David Dixon (PI)
Project Period: 10/01/2014 – 9/30/2015
Annual funding: 1 month summer salary

Funding Source: NSF
Project Title: *Experimental and Theoretical Study of Ligand Steric Effects in Homogeneous Catalysis*
PI: K. Shaughnessy (PI), David Dixon (co-PI)
Project Period: 09/01/2011 – 8/31/2015 (1 year no cost extension)
Annual funding: $50K

Funding Source: DOE-EFRC
Project Title: *The Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)*
PI: K. Krista Walton (Georgia Tech, PI), David Dixon (co-PI)
Project Period: 08/01/2014 – 7/31/2018
Annual funding: $2,800K, $100K

Funding Source: Department of Energy/Office of Basic Energy Sciences/Chemical Sciences, Geosciences, and Biosciences Division
Title: Molecular Mechanisms of Interfacial Reactivity in Near Surface and Extreme Geochemical Environments.
PI: Kevin Rosso (PNNL) D.A. Dixon
Project Period: FY2016-FY2018
Annual Funding: $2,321,000 ($60,000 to DAD)

Funding Source: Department of Energy/Office of Basic Energy Sciences/Chemical Sciences, Geosciences, and Biosciences Division
Title: Low-Temperature Catalytic Routes for Energy Carriers via Spatial and Chemical Organization
PI: Johannes Lercher (PNNL) D.A. Dixon
Project Period: FY2016-FY2018
Annual Funding: $6,397,000 ($105,867 to DAD)

Funding Source: NSF
Title: Use of Chromium(III) to Enhance the Protonation of Biomolecules by Mass Spectrometry
PI: Carolyn Cassady (UA) D.A. Dixon
Project Period: 07/01/2016 – 12/31/2019
Annual Funding: $150K

Funding Source: Department of Energy/Office of Basic Energy Sciences/Chemical Sciences, Geosciences, and Biosciences Division
Title: Modular Approaches to "Click" Complexants for Chemoselective Minor Actinide
PI: Jesse Carrick, TN Tech D.A. Dixon
Project Period: 07/01/2016 – 12/31/2019
Annual Funding: $150K ($12.5K to DAD)

Funding Source: Sentient Corporation for the United States Army Space and Missile Defense Command (USASMDC) – Redstone Arsenal
Title: High Density Phase Changing Missile Fuel: SBIR II
PI: D.A. Dixon
Project Period: 6/1/2015 – 12/31/2017
Annual Funding: $261,776 (2 years)

Funding Source: Sentient Corporation for the United States Army Space and Missile Defense Command (USASMDC) – Redstone Arsenal
Title: High Density Phase Changing Missile Fuel: SBIR II
PI: D.A. Dixon
Project Period: 1/1/2018 – 9/30/2018
Annual Funding: $167K

Funding Source: Sentient Corporation for the United States Army Space and Missile Defense Command (USASMDC) – Redstone Arsenal
Title: High Density Phase Changing Missile Fuel: SBIR II
PI: D.A. Dixon
Project Period: 10/31/2018 – 10/31/2020
Annual Funding: $261,776 (2 years)

Funding Source: Department of Energy/Office of Basic Energy Sciences/Chemical Sciences, Geosciences, and Biosciences Division

Title: Molecular Mechanisms of Interfacial Reactivity in Near Surface and Extreme Geochemical Environments.
PI: Kevin Rosso (PNNL) D.A. Dixon
Project Period: FY2019-FY2021
Annual Funding: $2,800,0050 ($80,000 to DAD)

Funding Source: Department of Energy/Office of Basic Energy Sciences/Chemical Sciences, Geosciences, and Biosciences Division
Title: Transdisciplinary Approaches to Realize Novel Catalytic Pathways to Energy Carriers
PI: Johannes Lercher (PNNL) D.A. Dixon
Project Period: FY2019-FY2021
Annual Funding: $ 10,830,130 ($120,000 to DAD)

Funding Source: DOE-EFRC
Project Title: *The Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)*
PI: K. Krista Walton (Georgia Tech, PI), David Dixon (co-PI)
Project Period: 08/01/2018 – 7/31/2022
Annual funding: $2,800K, $120K

Funding Source: Department of Energy/Office of Basic Energy Sciences/Chemical Sciences, Geosciences, and Biosciences Division
Title: Computational Studies of Hydrolysis of Actinides as Initial Steps in Aggregation and Attaining High Actinide Oxidation States
PI: D.A. Dixon
Project Period: 6/1/2018-5/31/2021
Annual Funding: $145,333

Funding Source: NSF
Title: CC*Compute: Accelerating Advances in Science & Engineering at The University of Alabama
PI: Jeff Carver (UA) D.A. Dixon (co-PI)
Project Period: 7/1/2020 – 6/30/2022
Total Funding: $399,995

Computer Time and Experimental Access at the William R. Wiley Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory During Tenure at UA – EMSL is funded by DOE BER

Molecular Computational Studies In Environmental Chemistry, Geochemistry, and Biogeochemistry E. Bylaska PI FY2004-2006

Reliable Electronic Structure Prediction of Molecular Properties Dixon PI FY2004 -2006

Direct Dynamics Simulations: From Molecules to Macromolecules and Condensed Phases W. Hase PI FY2004 -2006

*Computational Design of Catalysts: The Control of Chemical Transformati*on Dixon PI FY2004 -2006

Reliable Relativistic Quantum Chemistry Calculations for Molecules with Heavy Elements W. A. DeJong PI FY2005-2007

NMR for Catalyst Studies C. Peden PI FY2005-2007

The Impact of Carbonate on Surface Protonation, Electron Transfer and Crystallization Reactions in Iron Oxide Nanoparticles and Colloids Dixon PI FY2007-2009

Reliable Electronic Structure Prediction of Molecular Properties S. Xantheas FY2007-2009

Capture and Reduction of Metal Ions out of the Environment by Biomolecular Systems R. Lins FY2007-2009

Computational Design of Catalysts: The Control of Chemical Transformation to Minimize the Environmental Impact of Chemical Processes Dixon PI FY2007-2009 (1,000,000+ node hours per year)

Molecular Computational Studies In Geochemistry and Environmental Chemistry J. Rustad PI FY2007-2009

NMR and Computational Studies of Chemical Transformations at Complex Interfaces Dixon PI FY2007-2009

^{13}C NMR Investigation of Occluded Carbonate in Aluminum (Oxy)Hydroxides J. F. Boilly PI FY2008 -2010

Studies on 1,2,3-trichloropropane (TCP) and its derivatives E. Bylaska PI FY2008-2010

Large-scale computational modeling of the chemical behavior of actinide elements at interfaces W. A. De Jong PI FY2009-2011

The Role of Interfacial Processes on Mineral Transformations in Wet Supercritical CO_2 A. Felmy PI FY2010

NMR and Computational Studies of Chemical Transformations at Complex Interfaces for Catalytic Applications Dixon PI FY2010-2012

Early Transition Metal Oxides as Catalysts: Crossing Scales from Clusters to Single Crystals to Functioning Materials C. Peden PI FY2010-2012

Computational Design of Catalysts: The Control of Chemical Transformation to Minimize the Environmental Impact of Chemical Processes Dixon PI FY2010-2012

The Role of Interfacial Processes on Mineral Transformations in Wet Supercritical CO_2 A. Felmy PI FY2011-13

Fundamental Studies of Water Splitting on Model TiO_2, RuO_2 and Mixed TiO_2-RuO_2 Catalysts Henderson FY2012-2104

Computational Catalyst Design: Controlling Chemical Transformations to Minimize Environmental Impact Dixon PI FY2013-2014 (3,000,000 node hours per year)

Well-defined Metal-Oxide Catalysts to Understand Fundamental Chemical Transformations C. Peden PI FY2013-2014

Computational Studies of Catalyzed Chemical Transformations of Biomass Dixon PI FY2014-2015

*In-situ MAS NMR Investigations on Catalytic Conversion of Biogenic Molecules in the Presence and Absence of Wate*r J.Z. Hu FY2014-2015

The Role of Interfacial Processes on Mineral Transformations in Wet Supercritical CO_2 A. Felmy PI FY2014-15

Well-defined Metal-Oxide Catalysts to Understand Fundamental Chemical Transformations C. Peden PI FY2015-2016

Understanding Water Splitting on Model Mixed Metal Oxide Photocatalysts M. Henderson PI FY2015-2016

Advancing Heterogeneous Catalysis of Routes for the Conversion of Complex Biogenic Feedstocks in Aqueous and Apolar Solvents D. Camaioni PI FY2016-2017

Computational Studies of Catalyzed Chemical Transformations of Biomass-Derived Intermediates Dixon PI FY2016-2017

Mineral Reactivity and Transformations in Adsorbed Water Films J. Loring PI FY2016-2017

Well-defined metal-oxide catalysts to understand fundamental chemical transformations of biomass-derived molecules Y. Wang FY2017

Computational Studies of Catalyzed Chemical Transformations of Biomass and Derived Intermediates Dixon PI FY2018

*Computational Studies of Nanoparticle Formation Leading to Mineralization and ab initio Thermodynamics Studies of Mineral*s Dixon PI FY2019

Computational Studies of Nanoparticle Formation and Bulk Properties for Biomineralization, Dixon PI FY2020-2021

DOE INCITE Program OLCF at ORNL

Computational Actinide Chemistry: Reliable Predictions and New Concepts Dixon PI FY2014-2016

Reliable Predictions of Actinide Chemistry at Different Scales Dixon PI FY2017-2018

Predictive chemistry of realistic systems for advanced nuclear energy, Dixon PI FY2020