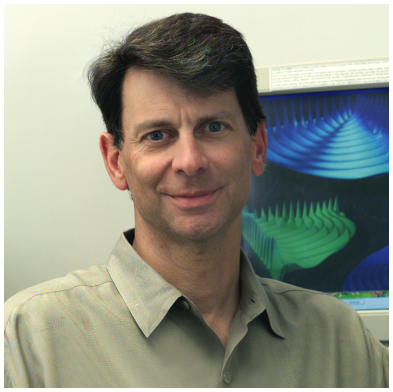
Dr. C. WILLIAM McCURDY, JR.

CURRICULUM VITAE

Summary

C. William McCurdy is a chemical physicist at the Lawrence Berkeley National Laboratory and the former Associate Laboratory Director for Computing Sciences. Dr. McCurdy is also a Professor in the Department of Applied Science, University of California, Davis, and Adjunct Professor of Chemistry at the University of California, Berkeley.



Before joining Lawrence Berkeley National Laboratory, he served as the founding director of the Ohio Supercomputer Center, while a member of the faculty in Chemistry at Ohio State University. From 1991 to 1995 he was the Director of the National Energy Research Supercomputer Center at Lawrence Livermore National Laboratory. He is a Fellow of the American Physical Society and has been a Camille and Henry Dreyfus Teacher-Scholar and an Alfred P. Sloan Research Fellow.

His research interests principally concern the theory of dynamical processes in chemistry and chemical physics. He has developed new fundamental methods for calculations on the basic processes of electron-driven chemistry including electron-molecule scattering, electron-impact ionization and molecular photoionization, and is the author of numerous publications in these areas.

Born March 21, 1949, in Atlanta, Ga., he received his B.S. (1971) from Tulane University and his Ph.D. in chemistry (1976) from the California Institute of Technology. In addition to English, he speaks fluent Spanish.

Address: One Cyclotron Road, MS: 50B-4230
Berkeley, California 94720

Telephone: (510) 486-4283

Current Positions

July 2004 - present	Professor, University of California, Davis, Departments of Applied Science (since 1991) and Chemistry (since 2004)
October 1996 - present	Adjunct Professor of Chemistry, Department of Chemistry, University of California, Berkeley

Past Professional Experience (in reverse chronological order)

December 1995 – October 2003	Associate Laboratory Director for Computing Sciences, and Senior Scientist, Lawrence Berkeley National Laboratory
January 2003 – April 2003	Visiting Professor at Universidad Autonoma de Madrid, Spain

July 1991- November 1995	Director, National Energy Research Supercomputer Center, Lawrence Livermore National Laboratory
May 1994 - October 1995	Acting Associate Director for Computations, Lawrence Livermore National Laboratory
October 1988 - July 1991	Professor of Chemistry, Ohio State University
April 1988 - March 1989	Visiting Scientist at Lawrence Livermore National Laboratory (Official LLNL title: "Participating Guest")
October 1987 - April 1988	Acting Director, Ohio Supercomputer Center
October 1986 - Sept. 1987	Acting Director, Ohio Supercomputer Project
November 1982 - Nov. 1985	Camille and Henry Dreyfus Teacher-Scholar
October 1983 - October 1988	Associate Professor of Chemistry, Ohio State University
January 1983 - June 1983	Visiting Professor at FOM Instituut voor Atoom en Molecuulfysica, Amsterdam-Watergraafsmeer, The Netherlands
April 1981 - 1983	Alfred P. Sloan Research Fellow
October 1978 - October 1983	Assistant Professor of Chemistry, Ohio State University

Education

July 1976 - July 1978	Postdoctoral study at University of California, Berkeley, with Professor W. H. Miller
December 1975- July 1976	Postdoctoral study at Cambridge University, Department of Theoretical Chemistry, with W. H. Miller, funded by NSF Energy-Related Postdoctoral Fellowship December 1975 - December 1976
1971-1975	California Institute of Technology, Pasadena, California, Ph.D. in Chemistry completed November 1975, Research director: Professor Vincent McKoy. Thesis title: *The Application of Basis Set Methods and Many-Body Theory in Electron-Molecule Scattering.* Earl C. Anthony Fellowship,

	Cal Tech, 1971-72, 1973-75, NSF Traineeship, Cal Tech, 1972-73, Teaching Assistant, Cal Tech, 1973-74.
1967-1971	Tulane University, New Orleans, Louisiana. B.S. (Chemistry) June 1971, Summa Cum Laude. Undergraduate research directed by Professor L. Chopin Cusachs, NSF Undergraduate Research Program Participant (1968, 1969, 1971)
- 1967	The Public Schools of Stone Mountain, Georgia

Professional Societies, Honors

Fellow of the American Physical Society - 1993
Ohio State University Distinguished Scholar Award - 1984
Alfred P. Sloan Research Fellow 1981 - 1983
Camille and Henry Dreyfus Teacher-Scholar Award - 1982
NSF Postdoctoral Fellowship, December 1975 - December 1976
Scientific Research Society of America, New Orleans Branch Gold Medal Award (1971) for undergraduate research
Sigma Xi
Phi Beta Kappa

Brief Description of Research Interests

Dr. McCurdy's principal areas of interest concern dynamical processes in chemistry and chemical physics. His work is both theoretical and computational, and exploits modern scalable supercomputing methods. Currently, the central topics being actively investigated are related to the development of techniques for calculations on electron-molecule scattering and molecular photoionization -- both with emphasis on polyatomic molecules. Another primary topic under current investigation is the theoretical and computational description of electron-impact ionization of atoms and molecules. Some specific topics on which work has been recently published or is in progress include:

- Low and high energy electron-molecule and electron-atom scattering, using finite basis set techniques and hybrid techniques including the complex Kohn method developed for polyatomic targets by Dr. McCurdy and his coworkers.
- Electron-impact ionization of atoms, including new mathematical and algorithmic approaches to first-principles calculations of detailed cross sections.
- Vibrational excitation by electron impact and dissociative attachment of electrons to polyatomic molecules.
- Valence shell multiple photoionization of atoms and molecules.

Selected Professional Service Activities – Federal Advisory Committees, Department of Energy

Basic Energy Sciences Advisory Committee (BESAC), 1998 – present.

Fusion Energy Sciences Advisory Committee (FESAC), 2000 – 2002.

Selected Professional Service Activities in High Performance Computing

NERSC Users Group (NUG); 1991- present.

NUG Executive Committee (NUGEX); 1991 - present.

DOE Scientific Computing Information Exchange; 1992 - 1997.

Coalition of Academic Supercomputing Centers (CASC) (Established 1989); 1993-present.

Committee of visitors, NSF program review, Division of Advanced Scientific Computing, Washington D.C., November 1993.

Systems of Lab's Computing Coordinating Committee (SLCCC) for the Department of Energy; 1994 - present.

Coordinating Committee for Informatics Research, Development and Application; 1993 - 1994.

Advisory Committee on Molecular Sciences Computing Facility, Pacific Northwest National Laboratory; 1994 - 1997.

University of Minnesota Supercomputing Institute's National National Advisory Board; 1996 - 1997.

University of Minnesota Supercomputing Institute's Digital Technology; 1997.

Strategic Simulation Plan (SSP), Department of Energy Working Group; 1997 – 2000

Co-Chair of the Steering Committee on Computational Physics (with R. Sugar), National Science Foundation, Division of Physics 2001-2002, organized NSF workshop, September 11-12, 2001, producing the NSF report, "Computation as a Tool for Discovery in Physics"

Chair of the organizing committee for the DOE Basic Energy Sciences workshop in May 2002, "Theory and Modeling in Nanoscience," producing the DOE published report with the same title.

Selected Professional Service Activities in Chemistry and Physics

Referee for Physical Review A, Journal of Chemical Physics, Chemical Physics, Chemical Physics Letters, Journal of the American Chemical Society, Journal of Computational Physics, and others.

Reviewer for National Science Foundation, Department of Energy

Member: Committee on Atomic Molecular and Optical Sciences (CAMOS), National Research Council, 1994 - 1997

The American Physical Society (APS) - Few-Body Systems & Multiparticle Dynamics Topical Group Nominating Committee, 1997 - present.

Chair of Steering Committee, and organizer of the National Science Foundation Workshop on Computational Physics, "Computational as a Tool for Discovery in Physics." NCSA, Arlington, VA, September 11-12, 2001.

Chair and organizer of the Workshop on "Theory and Modeling in Nanoscience," San Francisco, CA, May 10-11, 2002, Workshop conducted by the Basic Energy Sciences and Advanced Scientific Computing Advisory Committees to the Office of Science Department of Energy.

Co-chair of the Subcommittee on Theory and Computation in Basic Energy Sciencies – DOE Basic Energy Sciences Advisory Committee (BESAC) – 2003 – present.

Selected Service Activities at Lawrence Berkeley National Laboratory

Director's Action Committee (DAC), 1995 - present

Laboratory Directed Research and Development (LDRD) Proposal Evaluation Committee for Computational Sicence, 1995 - present

Environmental Council, 1997 - 1998

Computational Science Advisory Board, 1997

Physical & Chemical Biology Division Committee, 1997

Recent University Service Activities at the University of California, Davis

Ad Hoc Committee(s) for faculty merit/promotion process, Office of the Provost, UC Davis, 1997 - present

Member of Committee for the Initiative on Computational Science and Engineering, UC Davis, 1998-1999.

Chair, Search Committee for Faculty Position in Advanced Computational Engineering, Department of Applied Science, Livermore, CA., 1998.

History of Grant and Contract Support in Chemistry and Chemical Physics

Ohio State University Small Research Grant: "Classical Model for Electronic Degrees of Freedom in Non-Adiabatic Collisions," $4500 for academic year 79-80.

National Science Foundation Grant No. CHE-7907787. "Extension of Complex Coordinate and Complex Basis Function Techniques to Molecular Systems: Resonances and Photoionization." $118,000 three year continuing grant beginning November 1979.

Lawrence Livermore Laboratory Contract: "Development and Installation of Hartree-Fock Codes for Bound and Resonance Electronic States" with Professor Russell Pitzer, $9,372 for 6 months beginning June 1980.

Sloan Fellowship Award, $20,000 for two years beginning November 1981.

National Science Foundation, "Resonance Phenomena in Electron-Molecule Collisions," $185,000 three year continuing grant beginning November l982.

Camille and Henry Dreyfus Teacher-Scholar Award, $50,000, 1982.

Ohio State University Distinguished Scholar Award, $20,000, 1984.

National Science Foundation, "Photon- and Electron-Molecule Collisions and Molecular Resonance Phenomena," $184,000 three-year continuing grant beginning June 1986, CHE-8607496.

National Science Foundation, "Electron-Polyatomic Molecule Collisions and Ionization in Intense Fields," CHE-8922836, $202,500 three-year continuing grant beginning April 1990.

Spanish Ministry of Education and Culture: "Ayuda para estancias de Profesores, Investigadores, Doctores y Tecnologos Extranjeros en España," with Fernando Martín, Universidad Autonoma de Madrid, Spain, 11.000 euros, 2003.

Department of Energy, Lawrence Berkeley National Laboratory, Laboratory Directed Research and Development (LDRD):

- "Electron Collisions with Molecules and Clusters, and Surfaces," $190,000, June 1996-October 1997.
- "Electronic Collisions with Molecules and Clusters, and Surfaces," $190,000, October 1997-October 1998.
- "Electronic Collisions with Molecules and Clusters Above the Ionization Threshold," $220,000, October 1998 - October 1999.
- "Electron Collision Processes Above the Ionization Threshold," $200,000, October 1999-October 2001.
- "Scalable Methods for Studying Collisional Breakup and Rearrangement Processes," $110K, October 2001-October 2002.
- "Scalable Methods for Studying Collisional Breakup and Rearrangement Processes," with T. N. Rescigno, $130,000, October 2002.
- "Advanced Computational Methods for Photon-Molecule Collision Processes," with T. N. Rescigno, $175,000, October 2003.

Department of Energy Grant from Basic Energy Sciences: "Electron-Driven Chemistry", with T. N. Rescigno, $260,000 per year, December, 2000 – present (FY2003).

Summary of Activities in the Field of High Performance Computing in the National Laboratories

As Associate Laboratory Director for Computing Sciences at Lawrence Berkeley National Laboratory, Dr. McCurdy recently headed an organization with a total of more than 450 employees. The sum of the DOE funded budgets for these programatic activities is approximately $70M, and Dr. McCurdy was additionally responsible for approximately $40M of LBNL internally funded infrastructure activities. His activities in high performance computing in the Department of Energy National Laboratories began in 1991 at the DOE National Laboratory operated by the University of California in Livermore. Below is a short summary of his activities in the DOE labs.

As Director of the National Energy Research Supercomputer Center (NERSC) at Lawerence Livermore National Laboratory between July 1991 and November 1995, Dr. McCurdy was responsible for managing, providing general intellectual direction, and maintaining the budget of an enterprise funded at levels in excess of $38,000,000. The Energy Sciences Network (ESnet) was part of the responsibility of the Center. The Center's staff numbered in excess of 110 computing professionals, scientists, engineers and mathematicians. NERSC at Livermore was chartered to provide computational and international networking resources to researchers in Department of Energy (DOE) laboratories and in universities funded by the Energy Research programs of the DOE, as well as to carry out research in selected areas of the computational sciences. The Center served roughly two thousand users, about two-thirds in the DOE national laboratories and a third in universities nationwide.

Under Dr. McCurdy's direction the NERSC Center passed a number of significant milestones and accomplishments. He guided it through the conversion of all NERSC supercomputers to UNIX-based, vendor-supported operating systems in 1992, and moved the Center away from writing its own operating systems. He introduced massively parallel computing, with the acquisition of a Cray T3D, in 1994.

Under Dr. McCurdy's direction the budget of the facility grew to exceed $45,000,000 in Fiscal Year 1995, and its activities were extended to include existing applied mathematics programs at Livermore. Dr. McCurdy also served as Acting Associate Director for Computation at the Lawrence Livermore National Laboratory.

In December 1995, Dr. McCurdy joined the Lawrence Berkeley National Laboratory as Associate Laboratory Director for Computing Sciences. In November, 1995, the Department of Energy had made the decision to establish the NERSC and ESnet programs at LBNL under a new model for their relationship to the DOE laboratory and university research communities. In particular, NERSC at LBNL is responsible for long-range direct collaborations with major user groups and extensive support of the DOE Grand Challenge applications. In this role he is responsible for three Divisions of the Laboratory, the NERSC Center Division (a national unclassified high-performance computing user facility supported by DOE's Office of Science. NERSC currently provides computing resources to 2,100 users at national laboratories, research

centers and universities across the country), and the Computational Research Division (which carries out computational science, computer science and applied mathematics research and development in high-performance computing and distributed systems), and the Information Technologies and Services Division (which includes networking and distributed computing research supporting electronic technologies for scientific collaboration, the LBNL computing infrastructure, networking and telecommunications, computer protection and the Energy Sciences Network (ESnet). Dr. McCurdy is also responsible for the Applied Mathematics Department. The Computing Sciences Organization comprises more than 450 employees overall.

He reestablished the Center at Lawrence Berkeley National Laboratory in 1996, hiring a new staff of nationally recognized scientists and professionals (nearly half of whom are Ph.D.s), and building new computing resources including the Cray T3E massively parallel computer. In 1998 the largest computer at NERSC was upgraded to a T3E-900 with 640 processors, and NERSC staff members won Gordon Bell and Sid Fernbach awards.

In 1999, an IBM SP was added to the facility which was the first phase of the new five teraflop/s machine. Also in 1999, ESnet enhanced its services in a new partnership with Qwest. In 1999 the Laboratory undertook expanded computer security activities in all areas, including local and national networking services.

In 2000, a new 20,000 ft^2 computing facility in Oakland (the LBNL "Oakland Scientific Facility") was completed under Dr. McCurdy's direction. One of the largest computing facilities in the U.S. that includes offices and 6 Megawatts of power capability, this is the Laboratory's new computing facility that houses both NERSC and much of the LBNL computational infrastructure. In 2000, the NERSC center moved operations to the Oakland facility. The upgrade of the NERSC-3 computer, the IBM SP, to 3328 processors and 5.0 teraflop/s capability was initiated in this facility in January 2001. In November of 2002, the IBM system was upgraded to 6656 processors and 10.0 teraflop/s capability.

In early 2003, ESnet completed an upgrade to 2.5 gigabits (billions of bits or Gbps) per second and 10Gbps in the highest speed portions of the network that form its backbone.

Activities in the Field of High Performance Computing at the Ohio State University — 1984-1988

From 1984 to 1988, Dr. McCurdy devoted a portion of his efforts to establish a supercomputer facility at Ohio State University. As the Founding director of the Ohio Supercomputer Center he oversaw its establishment and secured the funding for both a Cray X-MP/24 and Cray Y-MP/864. A summary of that endeavor is given here.

Developing the proposals for the establishment of the Ohio Supercomputer Center

In 1984, Dr. McCurdy was a member of the committee to write the OSU proposal to National Science Foundation requesting funds to establish a national supercomputer center at Ohio State University. He then Chaired the *Ad hoc* Committee on Supercomputing from 1985 to 1987. This committee wrote the second proposal to NSF to establish a supercomputer training and graphics development center at Ohio State, as well as proposals for networking hardware. In this context his responsibilities included benchmarking of computer codes on various supercomputers, all contacts and negotiations with vendors, development of campus support, and coordination with office of the Vice President for Research and Graduate Studies, numerous trips to discuss proposals and networking issues at the National Science Foundation. He also coordinated these efforts with those of the Board of Regents of the State of Ohio to establish a statewide supercomputer center.

Administrative Positions in Computing at Ohio State University

Dr. McCurdy was the Acting Director of the "Ohio Supercomputer Project" from October 1, 1986, to October 1, 1987, when the Center was formally established. His responsibilities included the legislative interface and development effort with offices of the Governor of Ohio and members of the Ohio Legislature, coordination of efforts with the legislative liaisons for Ohio State and the Board of Regents, preparation of budgets and detailed plans for establishment of center, leading negotiation of the contract with Cray Research Incorporated for an X-MP/24 supercomputer, supervision of site preparation and installation of the first supercomputer, supervision of architectural plans and contracting for renovation of a building to house the supercomputer center, and development of job descriptions followed by hiring of the staff of the center. He also established the key committees which continued to govern and guide the Center for more than a decade following: the Governing Board, the Statewide Users' Group, and the Allocations Committee (Peer Review Group).

Upon funding by the Ohio Legislature, the "Project" became a "Center", and Dr. McCurdy was named the Acting Director of Ohio Supercomputer Center (Oct. 1 1987 to April 1, 1988). His responsibilities for the center included: budget authority for total funding of $16M for 1987-88 biennium, supervision of staff of 10-20 members during beginning months of operation, oversight of acceptance testing of the Cray X-MP/24 and UNICOS operating system, oversight or coordination of all committees listed above, and legislative relations efforts that secured $22M for next generation supercomputer to be purchased in 1989. He chaired the search committee to find a permanent Director for the facility, turned over its operation to the new Director on April 1, 1988, and returned to research and teaching at Ohio State.

From 1987 to 1989, Dr. McCurdy gave presentations, "The supercomputer revolution and the establishment of the Ohio Supercomputer Center" at various venues around the State of Ohio. He gave invited talks at international meetings on the process of establishing major computational facilities, for example, "Ohio: A Grass Roots Approach to Supercomputing," First Seminar on Supercomputer Applications, Universidad Nacional Autonoma de Mexico, Mexico City on September 7, 1989. He also gave public legislative testimony before: the Ohio House Select Committee on Technology on February 25, 1987, the Ohio House Finance and

Appropriations Committee on March 3, 1987, and Ohio Senate Finance Committee on May 12, 1987.

University Teaching Record

Courses Taught At Ohio State University

Year	Quarter	Course	Approx No. of Students
1978	Autumn	861 - Graduate Quantum Chemistry	5
1979	Winter	121 - General Chemistry	325
	Spring	996 - Seminar on Collision Theory	7
	Autumn	861 - Graduate Quantum Chemistry	5
1980	Winter	121 - General Chemistry	250
	Spring	533 - Physical Chemistry (undergrad)	110
	Autumn	861 - Graduate Quantum Chemistry	5
1981	Winter	121 - General Chemistry	250
	Spring	533 - Physical Chemistry	110
	Autumn	121 - General Chemistry	450
1982	Spring	882 - Graduate Statistical Mechanics	5
	Summer	694P – Spectroscopy	9
	Autumn	861 - Graduate Quantum Chemistry	8
1983	Summer	694P - Spectroscopy/Quantum Mechanics	9
	Autumn	H201 - Honors General Chemistry	60
1984	Winter	996 - Collision Theory	6
	Spring	882 - Statistical Mechanics	10
	Autumn	861 - Graduate Quantum Chemistry	20
1985	Winter	H202 - Honors General Chemistry	70
	Autumn	861 - Graduate Quantum Chemistry	20
1986	Winter	H202 - Honors General Chemistry	50
	Spring	882 - Statistical Mechanics	10
	Autumn	861 - Graduate Quantum Chemistry	25
1987	Spring	882 - Statistical Mechanics	10
1989	Spring	996 - Collision Theory	10
	Fall	861 - Graduate Quantum Chemistry	20
		H201 -Honors Freshman Chemistry	30
1990	Spring	531 - Physical Chemistry	55

	Fall	861 - Graduate Quantum Chemistry	15
1991	Winter	520 - Physical Chemistry (Thermodynamics)	55
	Spring	531 – Physical Chemistry	60

Courses Taught at Department of Applied Science, University of California, Davis

1992	Spring	228A - Properties of Matter (Statistical Mechanics)	9
1998	Autumn	EAL 230A - Quantum Mechanics	9
2001	Autumn	EAD 289A – Quantum Mechanics	10

Courses Taught at Department of Chemistry, University of California, Davis

2004	Fall	2A – General Chemistry	346

Courses Taught at Department of Chemistry, University of California, Berkeley

2005	Spring	221B – Advanced Quantum Mechanics	18

Patent

R.L. McCreery, C.W. McCurdy and P. Rossi, Diffractive Spectroelectro-chemistry, U.S. Patent 4395312, July 26, 1983.

Some Seminars, Lectures, Presentations and Workshops **in Chemistry and Physics**

"A New Helicity Representation for Reactive Atom-Diatom Collisions," American Chemical Society Symposium on State-to-State Chemistry, New Orleans, Louisiana, March 1977.

Invited talk: "Progress Toward the Application of Complex Coordinate and Complex Basis Function Techniques to Molecular Resonance Calculations," Asilomar Conference on Electron- and Photon-Molecule Collisions, August 1978.

Invited talk: "Complex Basis Function Calculations of Resolvent Matrix Elements." Special Session on topics in Mathematical Physics of the American Mathematical Society meeting, Boulder, Colorado, March 1980.

Departmental seminar: "Autoionizing States and Temporary Negative Ions: Bringing a Scattering Problem into the Realm of Quantum Chemistry":

Ohio University, Chemistry Department, Athens, Ohio, February 1980.
Washington University, Chemistry Department, St. Louis, MO, April 1980.
Illinois Institute of Technology, Chemistry Department, Chicago, Illinois, October 1980.
University of Illinois, Chemistry Department, Physical Chemistry Division, Urbana, Illinois, September 1981.
Purdue University, Chemistry Department, Physical Chemistry Division, West Lafayette, Indiana, November 1981.

Invited talk: "Extension and Application of Complex Scaling in Electron Scattering," Gordon Conference on "Few Body Problems in Chemistry and Physics," Brewster Academy, Wolfboro, New Hampshire, August 1981.

Departmental Seminar: "Atomic and Molecular Phenomena: New Theoretical Approaches," University of Nebraska, Physics Department, October 1982.

Physics Colloquium: "New Theoretical Approaches to Molecular Resonances," Universitat Bielefeld, West Germany, April 1983.

Physics Colloquium: "Wigner R-matrix Implementation of the CCGM Approximation for Surface Diffraction" - Max Planck Institut fur Stromungsforschung, Gottingen, West Germany, April 1983.

Physics Colloquium; "Electronic and Vibrational Motion in Resonant Electron-Molecule Collisions" - FOM-Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands, May 1983.

Physics Colloquium: "New Theoretical Approaches to Molecular Resonances" - Department of Physics, Albert Ludwigs Universitat, Freiberg, West Germany, May 1983.

Invited talk: "Resonance Phenomena in Election-Molecule Scattering," 8th Canadian Symposium on Theoretical Chemistry, Halifax, Nova Scotia, August 1983.

Departmental Seminar: "New Theoretical Approaches for Electron Scattering Resonances," University of Kentucky, Lexington, KY, Nov. 1983.

Invited talk: "Direct Variational Methods for Complex Resonance Energies," at the Symposium on Resonances, American Chemical Society National Meeting, St. Louis, MO, April 1984.

Departmental Seminar: "Distortions of the Energy Spectrum in Practical Calculations on Resonant and Nonresonant Scattering," James Franck Institute, University of Chicago, May 1984.

Departmental Seminar: "New Theoretical Methods for Molecular Resonances," Tulane University, November 1984.

Physical Chemistry Colloquium: "Local Complex Distortions of the Energy Spectrum in Scattering Calculations," University of Cincinnati, February 1985.

Physical Chemistry Colloquium: "New Theoretical Approaches for Molecular Photoionization and Metastable States," University of Pittsburgh, September 1985.

Physical Chemistry Colloquium: "Practical Calculation of Molecular Photoionization Cross Sections Using Local Complex Distortions of the Energy Spectrum," Los Alamos National Laboratory, November 1985.

Contributed Paper: "Molecular Photoionization Cross Sections by the Complex Basis Function Method," Fourteenth International Conference on the Physics of Electronic and Atomic Collisions," Palo Alto, California, July 1985.

Contributed Paper; "Calculation of Inelastic Electron-Atom Scattering Amplitudes by the Method of Locally Complex Distortions of the Energy Spectrum," Fourteenth International Conference on the Physics of Electronic and Atomic Collisions," Palo Alto, California, July 1985.

Invited Talk: "Molecular Photoionization Cross Sections by the Method of Complex Basis Functions," Midwest Theoretical Chemistry Symposium, Blomington, Indiana, May 15-16 1986.

Invited Talk: "Local Complex Distortions of the Energy Spectrum and Molecular Photoionization Calculations," Sanibel Symposium, Marineland, Florida, March 10-15 1986.

Contributed Paper: "Rigorous Method Using Square-Integrable Basis Functions for Calculation of Angular Dependence of Photoionization Cross Sections," Poster at Gordon Conference on Electron Spectroscopy, Wolfeboro, New Hampshire, July 14-18 1986.

Physics Colloquium: "Local Complex Distortions of the Energy Spectrum in Scattering Calculations," FOM Institute for Atomic and Molecular Physics, August 1986.

Invited Talk: "Complex Basis Set Techniques in Photoionization and Electron-Molecule Scattering Calculations," American Conference on Theoretical Chemistry, Gull Lake, Minnesota, July 25-31 1987.

Invited Talk: "Resonance and Threshold Features in Ab-Initio Calculations of Photoionization Cross Sections for Polyatomic Molecules," American Chemical Society 194th National Meeting, New Orleans, August 30 - September 4, 1987.

Physics Colloquium: "Local Complex Distortions of the Energy Spectrum in Photoionization," Physics Department, V-Division, Lawrence Livermore National Laboratory, April 1988.

Department Seminar: "New Theoretical Methods for Photoionization and Electron Scattering in Polyatomic Systems," Chemistry Department, University of Southern California, December 1988.

Theoretical Chemistry Seminar: "Electron-Polyatomic Molecule Scattering: New Methods and New Results," University of California-Berkeley, March 1988.

Work in Progress Seminar: "Accurate Treatment of Electron-Formaldehyde Elastic Scattering," V- Division, Lawrence Livermore National Laboratory, March 1988.

Contributed Paper: "*Ab Initio* Variational Techniques for Electron Collisions with Polyatomic Molecules," American Physical Society, Meeting of the Division of Atomic, Molecular and Optical Physics, Windsor, Ontario, May 1989.

Contributed Paper: "New Algebraic Variational Techniques for Electronic Collisions with Polyatomic Molecules," Poster, International Conference on the Physics of Electronic and Atomic Collisions, New York, July 1989.

Contributed Paper: "Theoretical Study of Electron Scattering by Formaldehyde," Poster, International Conference on the Physics of Electronic and Atomic Collisions, New York, July 1989.

Chemistry Colloquium: "Electronic Collisions with Polyatomic Molecules, " Physical Chemistry Colloquium, Ohio State University, November 1989.

Physics Colloquium: "Electronic Collisions with Polyatomic Molecules," Department of Physcs, University of Oklahoma, April 1990.

Contributed Paper: "Elastic Scattering of Low Energy Electrons by Polyatomic Molecules: *Ab Initio* Studies with the Complex Kohn Method," Meeting of the Division of Atomic, Molecular and Optical Physics (APS), Monterey, California, May 1990.

Contributed Paper: “Close-Coupling Studies of Electron Impact Excitation of H_2,” Meeting of the Division of Atomic, Molecular and Optical Physics (APS), Monterey, California, May 1990.

Invited Talk: “Electron-Polyatomic Molecule Collisions,” American Conference on Theoretical Chemistry, San Diego, California, July 1990.

Physics Colloquium: “Solving the Schrodinger Equation using Complex Coordinate Contours,” Department of Physics, Ohio State University, October 1990.

Chemistry Colloquium: "Electronic Collisions with Organic and other Polyatomic Molecules: Advances in Understanding Basic Phenomena Important in Industrial Applications," U.C. Davis, November 1991.

Contributed Paper: "Theoretical study of low-energy electron-NH_3 scattering", Meeting of the Division of Atomic Molecular and Optical Physics (APS) Washington, D. C. April 1991.

Invited Talk: "Low-energy electron scattering from polyatomic molecules: the role of electron correlation," ICPEAC Satellite meeting on Swarms and Electron-Molecule Scattering, Bond University, Australia, July 1991.

Contributed Paper: "*Ab initio* studies of low-energy electron-ethane scattering with target response", Meeting of the Division of Atomic Molecular and Optical Physics (APS) Chicago, Illinois, May (1992).

Chemistry Colloquium: "Electronic Collisions with Polyatomic Molecules: Inelastic and Elastic Scattering and the Role of Electronic Correlation", Pacific Northwest Laboratory (Environmental Molecular Sciences Laboratory), August 1992.

Invited Talk: "Complex exterior scaling and absorbing potentials in scattering calculations", NATO ARW, "Grid Methods in Atomic & Molecular Quantum Calculations," Corte, Corsica, France, September-October (1992).

Invited Talk: "Electron-Impact Excitation of Methane," Workshop on Comparative Study of Current Methodologies in Electron-Molecule Scattering, Institute for Theoretical Atomic and Molecular Physics, Harvard, March 1993.

Contributed Paper: "Electronic Excitation and Dissociation of the Methane Molecule upon Electron Impact at Low Energies," Meeting of the Division of Atomic Molecular and Optical Physics (APS) Reno, Nevada, May 1993.

Invited Talk: "Recent Theoretical Results On Electron-Polyatomic Molecule Collisions," Internal Conference on the Physics of Electronic and Atomic Collisions, Aarhus, Denmark, - July 1993.

Invited Talk: "Electron Scattering from Polyatomic Molecules: Ab Initio Treatment of Electronic Inelasticity and Target Response" Bottcher Memorial Symposium, Oak Ridge, Tennesee, March 1994.

Contributed Paper: "Ab-inito Complex-Kohn calculations of low-energy electron scattering cross sections from the SO_2 molecule", Meeting of the Division of Atomic Molecular and Optical Physics (APS), Crystal City, Maryland, April 1994.

Contributed Paper: “Electron and Photon Molecule Collisions”, ICPEAC Satellite Meeting, Berkeley, California, July 1995.

Invited Talk: "Low-energy Electron Scattering from Polyatomic Molecules: The Role of Electron Correlation and the Interface with Quantum Chemistry", West Coast Theoretical Chemistry Conference, Berkeley, CA, - April 1996.

Invited Talk: “Electronic Collisions with Polyatomic Molecules: Ab Initio treatment of Elastic and Inelastic Processes” Theory Seminar, Chemistry Department, UC Berkeley, CA, - May 1996.

Contributed Paper: "An Approach to Electron Impact Ionization that Avoids the Three-Body Coulomb Asymptotic Form," Meeting of the Division of Atomic Molecular and Optical Physics (APS), Washington D.C., - May 1997.

Invited Talk: "An Approach to Electron Impact Ionization that Avoids the Three-Body Coulomb Asymptotic Form," ITAMP Workshop on Resonances and Fragmentation of Three-Body Systems, Harvard University, - July 1997.

Invited Talk: “An Approach to Electron Impact Ionization that Avoids the Three-Body Coulomb Asymptotic Forum”, Auburn, Alabama, - April 1998.

Contributed Paper: “Low-Energy Electron Collision Processes in CF_4 and BCl_3”, DAMOP98 Meeting of The American Physical Society, Santa Fe, NM, - May 1998.

Workshop Presentaton: “Electron and Photon Initiated Chemistry”, Lawrence Berkeley National Laboratory, Berkeley, CA, October 9 - 10, 1998.

Physics Colloquium: “Theory of Ionization of Atoms and Molecules by Electron Impact,” University of Nevada, Reno, NV, February 1999.

Invited Talk: “Singly-Differential Cross Sections for Electron Impact Ionization of Atomic Hydrogen,” DAMOP, Atlanta, GA, - March 1999.

Invited Talk: “Electron Impact Ionization Calculations Avoiding the Three-Body Coulomb Asymptotic Form,” 52nd Annual Gaseous Electronics Conference, Norfolk, VA, - October 1999.

Invited Talk: "Fundamental Challenges in Electron-Driven Chemistry" Atomic, Molecular, and Optical Physics (AMOP) Contractor's Meeting, Boulder, Co, - October 1999.

Physics Colloquium: "Solving a Long-Standing Fundamental Problem of the Quantum Mechanics of Atoms: Ionization by Electron Impact," University of California at Berkeley, CA – February 2000.

Invited Talk: "Fundamental Challenges in Electron Driven Chemistry," DOE Workshop, Stevens Institute of Technology, March 2000.

Contributed Paper: "Practical Methods for Studying Quantum Mechanical Breakup Problems," 2000 Annual Meeting of DAMOP, University of Connecticut, Storrs, Connecticut - June 2000.

Plenary Presentation: "Solving a Long-Standing Fundamental Problem of the Quantum Mechanics of Atoms: Ionization by Electron Impact," Krell Institute's Computational Science Graduate Fellowship 2000 Conference, Lawrence Berkeley National Laboratory, Berkeley, CA, - July 2000.

Seminar Presenation: "Collisional Breakup of Quantum Systems of Charged Particles." Supercomputing 2000, Dallas Convention Center, Dallas, TX, - November 2000.

Seminar Presentation: "Solving a Long-Standing Fundamental Problem of the Quantum Mechanics of Atoms: Ionization by Electron Impact." University of California, Davis, Department of Applied Science, Livermore, CA – November 2000.

Invited Talk: "Collisional Breakup in a Quantum System of Three Charged Particles," 2001 AAAS Annual Meeting and Science Innovation Exposition, San Francisco, CA – February 2001.

Seminar Presentation: "Theory of Collisional Breakup of a System of Three Charged Particles." Chemical Dynamics Symposium to Honor Professor William Miller, University of California at Berkeley, CA – March 2001.

Plenary Presentation: "Reducing Collisional Breakup of a System of Charged Particles to Practical Computation: Electron-Impact Ionization of Hydrogen." XXII International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC), Santa Fe, NM – July 2001.

Physics Colloquium: "Electron-Impact Ionization of Atoms: Finally Solving The Most Basic Example," Georgia Institute of Technology, Atlanta, GA – March 2002.

Physics Colloquium: "Electron-Impact Ionization of Atoms: Finally Solving The Most Basic Example, Tulane University, New Orleans, LA – March 2002.

Chemistry Colloquium: "Electron Driven Chemistry", Department of Chemistry, Georgia Institute of Technology, Atlanta, GA – September 2002.

Physics and Chemistry Colloquium: “Ionización de átomos por impacto con electrones: Resolviendo un problema básico después de cuarenta años de intentos ,” Universidad Autónoma de Madrid – April 2003.

Invited Talk: “Dissociative Attachment of Electrons to Water: An *ab initio* Study of the Electronic and Nuclear Dynamics,” Workshop on the Interaction of Slow Electrons with Molecular Solids and Biomolecules, Harvard-Smithsonian Center for Astrophysics – October 2003.

Invited Talk: “Atomic and Molecular Double Photoionization and Electron Impact Ionization from First Principles Computation,” APS March Meeting, Montreal – March 2004.

Selected Presentations Concerning High Performance Computing

“Advanced Software Technology: Grand Challenge Projects and Mass Storage Systems,” Association for Energy Systems Operations and Programing, Oak Ridge, TN, - 1992.

“Future of Centralized High Performance Computing,” presentation to NSF Blue Panel on High Performance Computing, Washington D.C., - March 1993.

Panel Chair, DOE workshop on Distributed Collaborative Research Environments, Washington, D.C., - December 1993.

Workshop on Massively Parallel Computing, Lawrence Livermore National Laboratory, Livermore, CA, - June 1994

“Computational Science at Lawrence Livermore National Laboratory”, presentation given to numerous visiting groups in 1994 and 1995 including the Galvin Task Force on the Future of the National Laboratories, Livermore, CA.

“Scientific Computing: Hitting the Wall or Breaking New Ground?”, Lawrence Berkeley National Laboratory Office, Washington, D.C., - June 1997

“The Future of Computing: Hitting the Wall or Breaking New Ground?”, presented at the 1997 Berkeley National Laboratory Open House, Berkeley, CA, - October 1997.

“Scientific Computing: Hitting the Wall or Breaking Through it?”, UC Davis, Davis, CA, - June 1998.

“Systems Architecture and Platform Strategies”, Department of Energy, Computer Science and Enabling Technologies (CSET) Workshop, Argonne National Laboratory, Willowbrook, IL, - July 1998.

“The National Energy Research Scientific Computing (NERSC) Center and Scientific Computation at LBNL”, Annual Users’ Meeting of the Advanced Light Source (ALS), Lawrence Berkeley National Laboratory, Berkeley, CA - October 1998.

Workshop Presentation: "Computational Challenges in Atomic and Molecular Physics," Workshop on Computational Challenges in Atomic and Molecular Physics, Institute for Theoretical Atomic and Molecular Physics at the Harvard-Smithsonian Center for Astrophysics, Harvard University, Cambridge, MA, - May 2000.

"The Future of High Performance Computing in Science and Engineering," IAP Day 2000, Department of Computer Science, University of California, Davis, Davis, CA - May 2000.

Workshop Presentation: "Algorithms and High Performance Computing," Few Body Workshop, U.S. Department of Commerce, National Institute of Standards and Technology, Gaithersburg, MD – November 2000.

"Supercomputing from Applications Perspective: The Scientist's Dilemma, National Academy of Engineering Symposium," Lawrence Berkeley National Laboratory, Berkeley, CA - June 2001.

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4. C. William McCurdy, J.H. Corrington, H.S. Aldrich and L.C. Cusachs, "Dipole Moments and Orbital Energies from ARCANA: A Semiempirical Molecular Orbital Calculation Program," Int'l. J. Quant. Chem. **V S**, 307 (1971).

5. C. William McCurdy, and L.C. Cusachs, "Simplification of the RPA Secular Equation," J. Chem. Phys. **55**, 1994-1995 (1971).

6. C. William McCurdy, L.C. Cusachs and H.S. Aldrich, "Una Theoria Cuantica de Saturacion," Afinidad **28**, 1171 (1971).

7. Clyde W. McCurdy, Jr. and Vincent McKoy, "Equations of Motion Method: Inelastic Electron Scattering for Helium and CO_2 in the Born Approximation," J. Chem. Phys. **61**, 2820-2826 (1974).

8. Thomas N. Rescigno, Clyde W. McCurdy, Jr. and Vincent McKoy, "Calculation of Helium Photoionization in the Random-Phase Approximation Using Square-Integrable Basis Functions," Phys. Rev. A 9, 2409-2412 (1974).

9. T.N. Rescigno, C.W. McCurdy and V. McKoy, "Discrete Basis Set Approach to Nonspherical Scattering," Chem. Phys. Lett. **27**, 401-404 (1974).

10. T.N. Rescigno, C.W. McCurdy, Jr. and V. McKoy, "A Relationship Between the Many-Body Theory of Inelastic Scattering and the Distorted Wave Approximation," J. Phys. B **7**, 2396-2402 (1974).

11. T.N. Rescigno, C.W. McCurdy, Jr., and V. McKoy, "Low-Energy Elastic e^- -H_2 Cross Sections Using Discrete Basis Functions," Phys. Rev. A **11**, 825-829 (1975).

12. Thomas N. Rescigno, Clyde W. McCurdy, Jr. and Vincent McKoy, "Discrete Basis Set Approach to Nonspherical Scattering. II." Phys. Rev. A **10**, 2240-2245 (1974).

13. T.N. Rescigno, C.W. McCurdy, Jr. and V. McKoy, "Ab-Initio Cross Sections for the Excitation of the $b^3\Sigma_u^+$ State of H_2 by Electron Impact in the Distorted Wave Approximation," J. Phys. B **8**, L433-L436 (1975).

14. C.W. McCurdy, Jr., T.N. Rescigno and V. McKoy, "A Many-Body Treatment of Feshbach Theory Applied to Electron-Atom and Electron-Molecule Collisions," Phys. Rev. A **12**, 406-412 (1975).

15. T.N. Rescigno, C.W. McCurdy, Jr., and V. McKoy, "Photoabsorption Cross Sections of Two-Electron Atoms by the Coordinate Rotation Method: Application to H^- and Several States of He," J. Chem. Phys. **64**, 477-480 (1976).

16. C.W. McCurdy, Jr., T.N. Rescigno and V. McKoy, "A Simple Method for Evaluating Low-Energy Electron-Molecule Scattering Cross Sections Using Discrete Basis Functions," J. Phys. B **9**, 691-698 (1976).

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