

• **PETER W. LANGHOFF** •

• **Home Site** •

5332 Renaissance Avenue, San Diego, California 92122-5632
858-587-0594, plangho1@san.rr.com

• **Work Site** •

Department of Chemistry and Biochemistry, University of California, San Diego
9500 Gilman Drive, La Jolla, California 92093-0365
858-822-3611, planghoff@mail.ucsd.edu

• **Education** •

Hofstra University, Hempstead, NY - B.S. in Physics
State University of New York, Buffalo, NY - Ph.D. in Theoretical Physics
Harvard University, Cambridge, MA - Postdoctoral Fellow in Theoretical Chemistry
University of California, San Diego, CA - NIH National Research Fellow in Biophysics

• **Professional Societies** •

American Physical Society, Atomic, Molecular, and Optical Physics and Chemical Physics Divisions
American Chemical Society, Physical, Theoretical, and Biophysical Chemistry Divisions

• **Research Interests and Publications** •

Topical Areas of Study: Atomic and Molecular Physics; Mathematical and Theoretical Physics; Chemical Physics; Optical Physics - Dispersion, Scattering, and Fluorescence; Time-Dependent Quantum Theory; Theory of Molecular Photoionization Spectroscopy; VUV and X-Ray Photon Science; Theory of X-Ray Fluorescence; Computational Quantum Chemistry; Classical and Quantum Molecular Dynamics Simulations of Matter; Structure and Dynamics of Fluorescent Proteins; Solar Photochemistry; Aeronautics and Astronautics; Molecular Astrophysics, Reacting Flow Fields, Flow Field Visualization.

Publication Journals: Proceedings of the National Academy of Science (US), Reviews of Modern Physics, Physical Review, Physical Review Letter, Journal of Physical and Chemical Reference Data, Journal of Chemical Physics, Chemical Physics, Chemical Physics Letters, Journal of Mathematical Physics, International Journal of Quantum Chemistry, Journal of Electron Spectroscopy and Related Phenomena, Journal of Physical Chemistry A and B, Journal of Molecular Structure: THEOCHEM, Journal of Physics A and B, Journal of the Optical Society of America, Molecular Physics, Journal of Computational Physics, Physica Scripta, Journal de Chemie Physique, Journal of Molecular Science (China), American Journal of Physics, Computer Physics Communications, American Institute of Aeronautics and Astronautics Journal, Theoretical Chemistry Accounts.

• **Sponsoring Agencies** •

National Science Foundation - Chemistry Division, International Programs Division; Department of Energy - Basic Energy Sciences, Energy Infrastructure; Department of Defense - Air Force Office of Scientific Research, Air Force Research Laboratory; Air Force Materials Command, WPAFB; National Aeronautics and Space Administration; National Institutes of Health; ACS Petroleum Research Fund; Research Corporation; North Atlantic Treaty Organization; Proctor and Gamble Foundation; Hughes STX Corporation; National Research Council.

• **Professional Experience** •

Presently, Senior NAS/NRS Research Associate, Department of Chemistry & Biochemistry, University of California, La Jolla, CA - Participates in collaborative research in theoretical and physical chemistry, including development of new methods for *ab initio* studies of electronic structures and potential energy surfaces of molecules and materials. Interacts with colleagues in the Chemistry & Biochemistry Department on aspects of protein science and with colleagues in Physics on aspects of visible, vuv, & x-ray photon and electron-impact processes.

Presently, Senior Scientific Consultant, Air Force Research Laboratory, Edwards AFB, CA - Participates in definition and implementation of High-Energy-Density-Matter Program for development of advanced fuels and propulsion technologies in support of Air Force space propulsion requirements. Cooperates in the scientific research activities of a team of co-workers in the physics and chemistry of high energy density matter, including cryogenic, chemical, solar, and nuclear driven propulsion methodologies.

Presently, Chief Scientific Officer, Spectral Associates, LLC, Boston, MA and San Diego, CA - Defines and directs the scientific research activities of a team of co-workers in devising new and novel methods for *ab initio* determinations of the chemical structures and electronic properties of molecules and materials of technological importance. Supervises development of computational software in the implementation of methodologies devised for these purposes. Represents the Company for scientific purposes and in fundraising and related administrative activities.

1996 to 2011, Senior Fellow, San Diego Supercomputer Center, University of California, La Jolla, CA - Performs theoretical and computational studies of the interactions of ultraviolet and x-ray radiation and matter, including particularly inelastic light scattering, polarization phenomena, non-dipole effects, and inner-shell dynamics, in support of concomitant experiments performed at the University of California Berkeley Advanced Light Source and the Argonne National Laboratory Advanced Photon Source.

1988 to 1996, Professor of Chemistry, Indiana University, Bloomington, IN - Lectures in and developments graduate and undergraduate courses in the physical sciences, prepares research grant proposals, supervises postdoctoral and graduate student research projects, engages in graduate-student recruiting and academic committee assignments, including University Computing Requirements and Graduate School Ph.D. Standards.

1986 to 1988, Technical Director; 1994 to 1995, Vice President of Research, Solar Reactor Technology, Inc., Miami, FL - Defines and directs space-power and solar technology research and development programs, coordinates effort between SRT staff at academic institutions and industrial laboratories, manages budget process for DoE, DoD and NASA contracts, prepares technical proposals and reports, and makes oral presentations to sponsoring agencies, to Board of Directors, and to Company stockholders.

1985 to 1986, Professor of Theoretical Chemistry and Founding Faculty Associate, Supercomputer Computations Research Institute, Florida State University, Tallahassee, FL - Assists in establishing and developing the Institute under Department of Energy and State of Florida sponsorship. Directs the Research Institute Planning and University Supercomputer Resources Allocation Committees, prepares technical reports and oral presentations to DoE and State of Florida sponsors. Supervises the installation of campus-wide Ethernet and related digital communications system.

1977 to 1984, Professor and Chairman, Program in Chemical Physics, Indiana University, Bloomington, IN - As Professor, lectures in and aids the development of graduate and undergraduate courses in the physical sciences. Prepares successful research grant proposals to the National Science Foundation (Chemistry, Physics, International Programs), the Department of Energy, the ACS Petroleum Research Fund, the Department of Defense, the National Aeronautics and Space Administration, the North Atlantic Treaty Organization, the Research Corporation, the Proctor and Gamble Foundation. Supervises postdoctoral and graduate student research projects. Holds academic committee assignments, including University Computing Requirements and Graduate School Ph.D. Standards. Helps to organize national and international programs and workshops in the pure and applied sciences and to edit published proceedings, including the first International Workshop on Molecular Astrophysics, and participates in defining workshops for establishment of the DoE-sponsored Berkeley Advanced Light Source. As Chair, holds overall academic administrative and budgetary responsibility, organizes graduate-student recruiting efforts, and directs development and coordination of academic curricula, standards, and seminar activity. Secures support from funding sources, and represents the program to deans and other university administrators.

1976 to 1982, Adjunct Research Scientist, University of California Lawrence Livermore Laboratory, Livermore, CA - Performs theoretical studies on atomic and molecular ionization processes of fundamental interest in the development of high-power excimer gas lasers in support of the Livermore/DoE laser fusion program, studies aspects of electron-molecule scattering processes, and develops computer codes for laser-related topics in the physical sciences.

1969-75, Assistant/Associate Professor of Theoretical Chemistry, Indiana University, Bloomington, IN - Lectures in and develops graduate and undergraduate courses in physical chemistry, molecular quantum mechanics, statistical mechanics, and elementary chemistry. Organizes and directs a research group in theoretical chemistry under the auspices of external funding agencies, and guides the research efforts of undergraduate and graduate students in a range of topics in physical chemistry and chemical physics.

1968 to 1969, Adjunct Research Scientist, Massachusetts Institute of Technology Lincoln Laboratory, Lexington, MA - Performs research in missile re-entry physics and chemistry, particularly of ion recombination chemistry in hot air wakes, high-power ir laser atmospheric propagation, aspects of high-altitude cloud release, and the kinematics of atmospheric re-entry.

1967 to 1969, Postdoctoral Fellow in Chemistry, Harvard University, Cambridge, MA - Performs collaborative research in physical chemistry and chemical physics, particularly of the interactions between radiation and matter, optical properties of materials, and of intermolecular potentials in support of concomitant experimental molecular beam studies.

1966 to 1967, Technical Intelligence Officer, Technical Intelligence Directorate, U.S. Army Missile Command, Huntsville, AL - Develops techniques for interpretation of technical intelligence from airborne optical and shipborne radar platforms, related written and oral report preparation, strategic missile threat definition, liaison to Nike-X Project Office, NASA Marshall Space Flight Center, CIA, and to USAF-Office of Foreign Technology.

1962 to 1965, Research Scientist, Cornell Aeronautical Laboratory (Calspan, Inc.), Buffalo, NY - Performs research and development of radar power-correlation interferometer, effects of random receiver noise on bi-static radar signal interpretation, novel techniques of materials processing employing high-power microwave radiation, and studies of atomic processes of atmospheric interest, including electron-molecule radiative attachment cross sections, and spectra of atomic free radicals trapped in low-temperature inert gas solid matrices.

• **Visiting Appointments and Fellowship Awards** •

2012, Senior National Research Council Associate, Department of Chemistry and Biochemistry, University of California, 9500 Gilman Drive, La Jolla, California 92093-0365.

1998-99, NIH National Research Service Fellow in Biophysics, Department of Pharmacology, University of California, 9500 Gilman Drive, La Jolla, California 92093-0365.

1992, NASA Stanford-Ames Faculty Fellow, Department of Aeronautics and Astronautics, Stanford University, Stanford, California 94305.

1991-92, Senior National Research Council Associate, Phillips Laboratory, Edwards Air Force Base, Edwards, California 93524-7680.

1991, 2005, and 2010, Visiting Scientist Award, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106.

1989-90, Visiting Scientist, Institute for Theoretical Atomic and Molecular Physics, Harvard University, 60 Garden Street, Cambridge, Massachusetts 02138.

1983, Visiting Professor, Department of Chemistry, University of British Columbia, Vancouver, British Columbia V6T 1Y6, Canada.

1983, Professeur Associé, Laboratoire des Collisions Atomiques et Moléculaires, Université Paris, 91405, Orsay Cedex, France.

1981, Visiting Professor, Department of Theoretical Chemistry, University of Sydney, Sydney, NSW, Australia 2006.

1980-85, NSF-International Programs Adjunct Scientist, Max Planck Institute for Physics and Astrophysics, Karl-Schwarzschild Strasse 1, 8046 Garching bei München, West Germany.

1978-79, Senior National Research Council Associate, NASA Ames Research Center, Mountain View, California 94035.

1975-76, JILA Visiting Fellow, Joint Institute for Laboratory Astrophysics, National Bureau of Standards and University of Colorado, Boulder, Colorado 80309.

• **Selected Publications** •

Computational Quantum Chemistry and Physics

M. Ben-Nun, J.D. Mills, R.J. Hinde, C.L. Winstead, J.A. Boatz, G.A. Gallup, and P.W. Langhoff, P.W. “Atomic Spectral-Product Representations of Molecular Electronic Structure: Metric Matrices and Atomic-Product Compositions of Molecular Eigenstates,” *J. Phys. Chem.*, **113**, 7687-7697 (2009).

P.W. Langhoff, R.J. Hinde, J.D. Mills, and J.A. Boatz, “Spectral-Product Methods for Molecular Electronic Structure Calculations,” *Theor. Chem. Accounts*, **120**, 199-213 (2008).

P.W. Langhoff, J.A. Boatz, R.J. Hinde, and J.A. Sheehy, “Atomic Spectral Methods for Molecular Electronic Structure Calculations,” *J. Chem. Phys.*, **121**, 9323-9342 (2004).

P.W. Langhoff, R.J. Hinde, J.A. Boatz, and J.A. Sheehy, “Applications of Löwdin’s Metric Matrix: Atomic Spectral Methods for Electronic Structure Calculations,” in *Fundamental World of Quantum Chemistry: A Tribute to the Memory of Per-Olov Löwdin*, edited by Erkki Brändas and Eugene S. Kryachko (Kluwer Academic, Dordrecht, 2004), Vol. 3, pp. 97-114. Invited contribution to Löwdin Memorial Volume.

P.W. Langhoff, R.J. Hinde, J.A. Boatz, J.A. Sheehy, “Spectral Theory of the Chemical Bond,” *Chem. Phys. Lett.* **358**, 231-236 (2002).

J. M. Spotts, C. K. Wong, M. S. Johnson, M. Okumura, J. A. Boatz, J. Sheehy, R. J. Hinde, and P. W. Langhoff, “Multiphoton Ionization Spectroscopy of $AlAr_N$ Clusters,” *J. Phys. Chem. A*. **107**, 6948-6965 (2003).

P.W. Langhoff, J.A. Boatz, R.J. Hinde, J.A. Sheehy, “Spectral Theory of Chemical Bonding,” in *Low-Lying Potential Energy Surface*, Hoffmann, M.R.; Dyall, K.G. Eds., ACS Symposium Series 828: Washington, DC, USA, 2002; Chapter 10, pp. 221-237.

P.W. Langhoff, “Spectral Theory of Physical and Chemical Binding,” *J. Phys. Chem.*, **100**, 2974-2984 (1996).

Atomic, Molecular, and Optical Physics

O. Hemmers, R. Guillemin, D. Rolles, A. Wolska, D.W. Lindle, E.P. Kanter, B. Krässig, S.H. Southworth, R. Wehlitz, B. Zimmermann, V. McKoy, and P.W. Langhoff, "Low-Energy Nondipole Effects in Molecular Nitrogen Valence-Shell Photoionization," *Physical Review Letters* **97**, 103006 (2006).

J.W. Cooper, C.H. Green, P.W. Langhoff, A.F. Starace, and C.L. Winstead, "Comment on Fano Lineshapes Revisited: Symmetric Photoionization from Pure Continuum Excitation," *Physical Review Letters* **94**, 229301 (2005).

P.W. Langhoff and C.L. Winstead, "Spectral Properties of Minimal-Basis-Set Orbitals: Implications for Molecular Electronic Continuum States," *Int. J. Quantum Chem.* **102**, 948-955 (2005). Invited contribution to Pople Memorial Volume.

R. Guillemin, O. Hemmers, D.W. Lindle, E. Shigemasa, K. LeGuen, D. Ceolin, C. Miron, N. Leclercq, P. Morin, M. Simon, and P.W. Langhoff, "Nondipole Electron Angular Distributions from Fixed-in-Space Molecules," *Phys. Rev. Lett.* **89**, 033002 1-4 (2002).

P.W. Langhoff, J.C. Arce, and J.A. Sheehy, "Dynamical Theory of Molecular Photoionization: Electron Ejection Dynamics and Angular Distributions from Molecules Fixed in Space," *J. Electron Spectro. & Relat. Phenom.* **123**, 117-132 (2002). Invited contribution to C.E. Brion Festschrift.

J.C. Arce, J.A. Sheehy, P.W. Langhoff, O. Hemmers, H. Wang, P. Focke, I.A. Selin, and D.W. Lindle, "On the Angular Distributions of Molecular Photoelectrons: Dipole Cross Sections for Fixed-in-Space and Randomly Oriented Molecules," *Chem. Phys. Lett.* **346**, 341-346 (2001).

P.W. Langhoff, J.C. Arce, J.A. Sheehy, O. Hemmers, H. Wang, P. Focke, I.A. Selin, and D.W. Lindle, "On the Angular Distributions of Electrons Photoejected from Fixed-in-Space and Randomly Oriented Molecules," *J. Electron Spectro. & Relat. Phenom.* **114-116**, 23-32 (2001).

O. Hemmers, H. Wang, P. Focke, I.A. Selin, D.W. Lindle, J.C. Arce, J.A. Sheehy, and P.W. Langhoff, "Large Nondipole Effects in the Angular Distributions of K-Shell Photoelectrons from Molecular N₂," *Phys. Rev. Lett.* **87**, 273003 1-4 (2001).

O. Hemmers, H. Wang, D.W. Lindle, P. Focke, I.A. Selin, J.D. Mills, J.A. Sheehy, and P.W. Langhoff, "Beyond the Dipole Approximation: Angular Distribution Effects in the 1s Photoemission from Small Molecules," in *X-Ray and Inner-Shell Processes, X-99*, R.W. Dunford, et.al., Editors (American Institute of Physics, Melville, NY, 2000).

J.D. Bozek, N. Berrah, E. Kukk, T.D. Thomas, T.X. Carroll, L.J. Saethre, J.A. Sheehy, and P.W. Langhoff, "High-Resolution Molecular Inner-Shell Electron Spectroscopies," in *X-Ray and Inner-Shell Processes, X-99*, R.W. Dunford, et.al., Editors (American Institute of Physics, Melville, NY, 2000), pp. 188-204,

E. Kukk, J.D. Bozek, T.D. Thomas, T.X. Carroll, L.J. Saethre, J.A. Sheehy, N. Berrah, and P.W. Langhoff, "New Insights into Molecular Structure and Dynamics Using Soft

X-Ray Electron Spectroscopy,” in *The Physics of Electronic and Atomic Collisions*, Y. Itikawa, et.al., Editors (American Institute of Physics, Melville, NY, 2000), pp. 163-171, K. Kukuk, J.D. Bozek, N.Berrah, J.A. Sheehy and P.W. Langhoff, “Angular Distributions of Molecular-Field and Spin-Orbit Split Core Levels of Sulfur 2p Photoionization in OCS,” *J. Phys. B* **33**, L51-L57 (2000).

Theory of Fluorescent Proteins

H.-Y. Yoo, J.A. Boatz, V. Helms, J.A. McCammon, and P.W. Langhoff, “Chromophore Protonation States and the Proton Shuttle Mechanism in Green Fluorescent Protein: Inferences Drawn from Ab Initio Theoretical Studies of Chemical Structures and Vibrational Spectra,” *J. Phys. Chem. B* **105**, 2850-2857 (2001).

V. Helms, C.L. Winstead, and P.W. Langhoff, “Low-Lying Electronic Excitations of the Green Fluorescent Protein Chromophore,” *Journal of Molecular Structure: THEOCHEM*, **506**, 179-189 (2000).

W. Weber, V. Helms, J.A. McCammon, and P.W. Langhoff, “Shedding Light on the Dark and Weakly Fluorescent States of Green Fluorescent Proteins,” *Proc. Natl. Acad. Sci.* **96**, 6177-6182 (1999).

V. Helms, E.F.Y. Hom, T.P. Straarsma, J.A. McCammon, and P.W. Langhoff, “Exciting Green Fluorescent Protein,” in *Combined Quantum Mechanical and Molecular Mechanical Methods*, J. Gao and M.A. Thompson, Editors, ACS Symposium Series 712 (American Chemical Society, Washington, DC, 1998), Chapter 19, pp. 288-295.

Air Force Research Laboratory Publications

Langhoff, P.W., Boatz, J.A., and Fajardo, M.E., “Theoretical Methods for Cryogenically Trapped Metal Radical Spectra,” *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Crystal Bay, Nevada, on June 5-7, 1994, pp. 229-237.

Mills, J.D., Larson, C.W., Erdman, P.S., Stwalley, W.C., and Langhoff, P.W., “Optical Absorption, Emission, and Radiation Trapping in High-Temperature Metal Vapors,” *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Crystal Bay, Nevada, on June 5-7, 1994, pp. 238-244.

Langhoff, P.W., “Spectral Theory of Chemical Bonding: Aggregates of Weakly Bound Atoms,” *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Woods Hole, Massachusetts, on June 4-7, 1995, pp. 93-98.

Boatz, J.A., Fajardo, M.E., and Langhoff, P.W., “Monte Carlo Simulations of the Structures and Optical Absorption Spectra of Na/Ar_N Clusters and Solids: An Application of Spectral Theory of Chemical Binding,” *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Woods Hole, Massachusetts, on June 4-7, 1995, pp. 99-113.

Mills, J.D., and Langhoff, P.W., “Theory of Laser Induced Fluorescence Lineshapes: Applications to Doped Cryogenic Clusters,” *Proceedings of the High Energy Density Matter*

(*HEDM*) Conference (9th), Held in Woods Hole, Massachusetts, on June 4-7, 1995, pp. 313-313.

Sheehy, J.A., Boatz, J.A., Fajardo, M.E., and Langhoff, P.W., "Spectral Theory of Weakly Bonded Atomic Aggregates," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Boulder, Colorado, on June 5-7, 1996, pp. 48-57.

Boatz, J.A., Fajardo, M.E., Sheehy, J.A., and Langhoff, P.W., "Monte Carlo Simulations of the Structures and Optical Absorption Spectra of Na/Ar Clusters and Solids: An Application of Spectral Theory of Chemical Bonding," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Boulder, Colorado, on June 5-7, 1996, pp. 165-174.

Langhoff, P.W., Boatz, J.A., and Sheehy, J.A., "Spectral Theory of Physical and Chemical Bonding: Aspects of Computational Implementation," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Chantilly, Virginia, on June 1-3, June 1997, pp. 82-90.

Sheehy, J.A., Boatz, J.A., Mills, J.D., and Langhoff, P.W., "Theoretical Investigations of HEDM," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Chantilly, Virginia, on June 1-3, June 1997, pp. 110-116.

Boatz, J.A., Sheehy, J.A., and Langhoff, P.W., "Monte Carlo Simulations of the Structures and Optical absorption Spectra of Al/Ar_N Clusters: Applications of Spectral Theory of Chemical Bonding," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Chantilly, Virginia, on June 1-3, June 1997, pp. 185-195.

Langhoff, P.W., "Spectral Theory of Adiabatic Electronic Schrödinger Eigenstates: Structure and Spectra of Al/Ar_N Cryogenic Clusters," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Monterey, California, on June 17-20, May 1998, pp. 39-43.

Boatz, J.A., Sheehy, J.A., and Langhoff, P.W., "Monte Carlo Simulations of the Structures and Optical Absorption Spectra of Al/Ar_N Clusters," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Monterey, California, on June 17-20, 1998, pp. 84-101.

Langhoff, P.W., "Spectral Theory of the Chemical Bond: Atomic-Based Formalism for Chemical Aggregates," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Cocoa Beach, Florida, on June 8-10, 1999, pp. 34-38.

Boatz, J.A., Sheehy, J.A., Hinde, R.J., and Langhoff, P.W., "Classical and Quantum Monte Carlo and Molecular Dynamics Simulations of the Structures, Photoinduced Fragmentation, and Optical Absorption Spectra of Al/Ar_N Clusters," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Cocoa Beach, Florida, on June 8-10, 1999, pp. 111-121.

Langhoff, P.W., Boatz, J.A., and Sheehy, J.A., "Spectral Theory of Chemical Bonding," *Proceedings of the High Energy Density Matter (HEDM) Conference*, Held in Park City, Utah, on October 24-26, 2000, pp. 44-44.

• Selected Invited Presentations (I) and Contributed Papers (C) •

“Molecular Structure and Spectra: Discrete and Continuum Electronic States of Molecules and Materials,” First Colombian School on Theoretical and Computational Methods in Molecular Science, 28 May to 3 June 2012, University del Valle, Cali, Colombia (I)

“Large-Scale Valence-Bond Calculations on Diatomic Molecules: Aspects of Spectral Compression,” American Physical Society Meeting, Division of Atomic, Molecular, and Optical Physics, Houston, TX, AZ, 25-29 May 2010 (C).

“Spectral Theory for Molecules and Materials,” American Physical Society National Meeting, Portland, OR, 30 March 2010 (C).

“Re-Examination of Fano Parameterization in Resonant Photoionization Theory,” American Physical Society Meeting, Division of Atomic, Molecular, and Optical Physics, Tucson, AZ, 28 May 2004 (C).

“Classical and Quantum Dynamics of Extended Systems,” 44th Sanibel Symposium on Theory and Computations in Molecular and Materials Sciences, Biology and Pharmacology, St. Augustine, FL, 3 March 2004 (I).

“Theory of Open-Shell Metal Atoms in Cryogenic Matrices,” 227th American Chemical Society National Meeting, Anaheim, CA, 30 March 2004 (C).

“Aspects of Molecular Photoionization,” Chemistry Division, Argonne National Laboratory, Argonne, IL, 27 October 2003 (I).

“Theoretical and Experimental Studies of Metal-Rare Gas Clusters,” Center of Bioinformatics, Saarland University, Saarbrücken, Germany, 22 July 2003 (I).

“Theoretical Studies of Fluorescent Proteins,” International Workshop on Protein Science, Abdus Salam International Center for Theoretical Physics, Trieste, Italy, 18 July 2003 (I).

“Theory of Metal-Rare Gas Cryogenic Clusters,” Dipartimento di Chimica, University of Rome, Rome, Italy, 11 September 2003 (I).

“Physical and Chemical Aspects of Fluorescent Proteins,” Department of Chemistry, University of Las Vegas, Las Vegas, NV, 24 April 2003 (I).

“Spectral Theory of Chemical Bonding,” in *Low-Lying Potential Energy Surfaces*, M. Hoffmann and K.G. Dyall, Editors (American Chemical Society Publication, Washington, DC, 2002), Chapter 10, pp. 221-237. ACS Symposium Address (I).

“On the Angular Distributions of Electrons Photoejected from Molecules” 221st American Chemical Society National Meeting, San Diego, CA, 1 April 2001 (C).

“Chromophore Charge States and the Proton Shuttle Mechanism in Green Fluorescent Protein,” 221st American Chemical Society National Meeting, San Diego, CA, 4 April 2001 (C).

“Structure and Spectra of Green Fluorescent Protein Chromophore,” 219th American Chemical Society National Meeting, San Francisco, CA, 28 March 2000 (C).

• **Comprehensive Publication List** •

- "Multipole Polarizabilities and Shielding Factors from Hartree-Fock Wave Functions," *The Physical Review* **139**, A1415 (1965), with R.P. Hurst.
- "Electric Dipole Hyperpolarizabilities for S-State Atoms and Ions," *The Physical Review* **148**, 18 (1966), with J.D. Lyons and R.P. Hurst.
- "Uniform-Electric-Field Quadrupole Polarizabilities and Shielding Factors for S-State Atoms and Ions," *The Physical Review* **151**, 60 (1966), with J.D. Lyons and R.P. Hurst.
- "Approximations to Hartree-Fock Perturbation Theory," *The Journal of Chemical Physics* **44**, 505 (1966), with M. Karplus and R.P. Hurst.
- "Bounds for van der Waals Coefficients from Padé Approximants," *Physical Review Letters* **19**, 1461 (1967), with M. Karplus.
- "Padé Summation of the Cauchy Dispersion Equation," *Journal of the Optical Society of America* **59**, 863 (1969), with M. Karplus.
- "Padé Approximants to the Normal Dispersion Expansion of Dynamic Polarizabilities," *The Journal of Chemical Physics* **52**, 1435 (1970), with M. Karplus.
- "Bounds for Oscillator-Strength Sums from Approximate Quadratures," *Physical Review Letters* **25**, 1317 (1970), with A.C. Yates.
- "Padé Approximants for Two- and Three-Body Dipole Dispersion Interactions," *The Journal of Chemical Physics* **53**, 233 (1970), with M. Karplus.
- "Comment on Chemistry of Electrons in Pure-Air Hypersonic Wakes," *American Institute of Aeronautics and Astronautics Journal* **8**, 382 (1970).
- "Application of Padé Approximants to Dispersion Force and Optical Polarizability Computations," in *The Padé Approximant in Theoretical Physics*, edited by G.A. Baker, Jr., and J.L. Gammel (Academic, NY, 1970), pp. 41-97, with M. Karplus.
- "Comparison of Dispersion Force Bounding Methods with Applications to Anisotropic Interactions," *The Journal of Chemical Physics* **55**, 2126 (1971), with R.G. Gordon and M. Karplus.
- "Bounds for Second-Order Optical Properties from Quantum-Mechanical Sum Rules and the Theory of Moments," *Chemical Physics Letters* **9**, 89 (1971).
- "Sum-Rule Moment Bounds on Long-Range van der Waals Potentials," *Chemical Physics Letters* **12**, 217 (1971).
- "Moment Theory Bounds on Long-Range Casimir-Polder Potentials," *Chemical Physics Letters* **12**, 223 (1971).
- "Schrödinger Particle in a Gravitational Well," *The American Journal of Physics* **39**, 954 (1971).
- "Moment Theory Bounds for the Second-Order Optical Properties of Atoms and Molecules," *The Journal of Chemical Physics* **57**, 2604 (1972).
- "Aspects of Time-Dependent Perturbation Theory," *Review of Modern Physics* **44**, 602 (1972), with S.T. Epstein and M. Karplus.

"Moment Theory Bounds On the Mean Energies of Stopping, Stragglng, and Molecular Excitation," *The Journal of Physics B* **5**, 1071 (1972), with A.C. Yates.

"Casimir-Polder Separation Theorem for Second-Order Coulomb Energies," *Chemical Physics Letters* **20**, 33 (1973).

"Stieltjes Imaging of Atomic and Molecular Photoabsorption Profiles," *Chemical Physics Letters* **22**, 60 (1973).

"Variational Approximations to Time-Dependent Hartree-Fock Theory," *Molecular Physics* **25**, 345 (1973), with S.W. Chan.

"Separation Theorem for First-Order Pair-Correlation Equations," *International Journal of Quantum Chemistry* **S7**, 443 (1973).

"Dispersion Theorem for the Thermodynamic Properties of Harmonic Crystals," *Molecular Physics* **26**, 203 (1973), with C.T. Corcoran.

"Stieltjes Imaging of Fredholm Determinants," *Chemical Physics Letters* **24**, 724 (1974), with W.P. Reinhardt.

"Stieltjes Imaging of Electron Impact-Excitation Profiles," *Chemical Physics Letters* **27**, 195 (1974), with S.L. Seidman.

"Stieltjes-Integral Approximations to Photoabsorption and Dispersion Profiles in Atomic Helium," *The Physical Review A* **10**, 829 (1974), with J. Sims and C.T. Corcoran.

"Stieltjes Imaging of Photoabsorption and Dispersion Profiles," *The Journal of Chemical Physics* **61**, 146 (1974), with C.T. Corcoran.

"Stieltjes-Integral Approximations to Elementary Dispersion Relations," *International Journal of Quantum Chemistry* **S8**, 347 (1974).

"Quantum Theory of Radiative Transition Phenomena," *International Journal of Quantum Chemistry* **S9**, 461 (1975), with W.R. Heffner.

Moment-Theory Investigations of Photoabsorption and Dispersion Profiles in Atoms and Ions," *The Physical Review A* **14**, 1042 (1976), with C.T. Corcoran, J.S. Sims, F. Weinhold, and R.M. Glover.

"Tchebycheff-Derivative Approximations to Photoabsorption Cross Sections in Atoms and Ions," *Chemical Physics Letters* **40**, 367 (1976), with C.T. Corcoran.

"Polynomial Expansions for Spectral Densities," *Chemical Physics Letters* **41**, 609 (1976), with C.T. Corcoran.

"On the Habitability of Mars," NASA Special Publication 414 (National Technical Information Service, Springfield, Virginia, 1976), 105 pages, with R.D. MacElroy, M.M. Averner, S. Berman, W.R. Kuhn, S.R. Rogers, and J.W. Thomas.

"Moment-Theory Approximations to Non-Negative Spectral Densities," *Journal of Mathematical Physics* **18**, 651 (1977), with C.T. Corcoran.

"On the Brueckner and Goldstone Forms of the Linked-Cluster Theorem," *International Journal of Quantum Chemistry* **S10**, 337 (1976), with A.J. Hernandez.

"Green's-Function Calculations of Ground-State Correlation Energies," *Chemical Physics Letters* **49**, 361 (1977), with A.J. Hernandez.

"On Rayleigh-Schrödinger and Green's Function Calculations of Ionization Potentials and Electron Affinities," *Chemical Physics Letters* **49**, 421 (1977), with A.J. Hernandez.

"Photoabsorption in Atomic Lithium," *The Physical Review A* **16**, 1513 (1977), with C.T. Corcoran and J.S. Sims.

"Moment-Trace Calculations of Atomic and Molecular Photoabsorption Cross Sections," *Chemical Physics Letters* **52**, 380 (1977), with P.M. Johnson, S.V. O'Neil, C.T. Corcoran, and W.P. Reinhardt.

"Applications of the Stieltjes-Tchebycheff Procedure for Atomic and Molecular Photoionization Calculations in Hilbert Space" *International Journal of Quantum Chemistry* **S11**, 301 (1977).

"Photoabsorption in Formaldehyde," *The Journal of Chemical Physics* **67**, 1722 (1977), with S.R. Langhoff and C.T. Corcoran.

"K-Shell Photoionization in N₂," *Chemical Physics Letters* **51**, 65 (1977), with T.N. Rescigno.

"Resonance Refractivity Studies of Sodium Vapor for Enhanced Flow Visualization," *American Institute of Aeronautics and Astronautics Journal* **16**, 1106 (1978), with D. Bershader and G. Blendstrup.

"Photoabsorption in Molecular Nitrogen," *The Journal of Chemical Physics* **68**, 970 (1978), with T.N. Rescigno, C.F. Bender, and B.V. McKoy.

"Photoabsorption in Carbon Monoxide: Stieltjes-Tchebycheff Calculations in the Separated-Channel Static-Exchange Approximation," *The Journal of Chemical Physics* **69**, 2992 (1978), with N. Padial, G. Csanak, and B.V. McKoy.

"Photoabsorption in Formaldehyde: Intensities and Assignments in the Discrete and Continuous Spectral Intervals," *The Journal of Chemical Physics* **69**, 4689 (1978), with A. Orel, T.N. Rescigno, and B.V. McKoy.

"Photoabsorption in H₂O: Stieltjes-Tchebycheff Calculations in the Time-Dependent Hartree-Fock Approximation," *Chemical Physics Letters* **60**, 201 (1979), with G.R.J. Williams.

"Photoionization in Molecular Oxygen," *International Journal of Quantum Chemistry* **S13**, 643 (1979), with A. Gerwer, C. Asaro, and B.V. McKoy.

"On II-Shell Photoionization in Molecular Nitrogen," *Chemical Physics Letters* **66**, 116 (1979), with T.N. Rescigno, A. Gerwer, and B.V. McKoy.

"The Stieltjes-Tchebycheff Moment-Theory Approach to Molecular Photoionization Studies," in *Electron-Molecule and Photon-Molecule Collisions*, T. Rescigno, B.V. McKoy, and B. Schneider, Eds. (Plenum, New York, 1979), pp. 183-224.

"Molecular Photoionization," in *Proceedings of the Caracas Symposium on Structure, Interactions, and Reaction Mechanisms in Chemistry* (Simon Bolivar UP, Caracas, 1980).

"Stieltjes-Tchebycheff Moment-Theory Approach to Photoeffect Studies in Hilbert Space," in *Theory and Applications of Moment Methods in Many-Fermion Systems*, edited by B.J. Dalton, S.M. Grimes, J.P. Vary, and S.A. Williams (Plenum, New York, 1980), pp. 119-212.

- "Theoretical Studies of Molecular Partial-Channel Photoionization Cross Sections," in *Molecular Physics and Quantum Chemistry Workshop*, edited by P.G. Burton (Wollongong U.P., Wollongong, 1980), Chapter 3, pp. 1-32.
- "Photoexcitation and Ionization in Molecular Oxygen; Theoretical Studies of Electronic Transitions in the Discrete and Continuous Spectral Intervals," *The Journal of Chemical Physics* **72**, 713 (1980), with A. Gerwer, C. Asaro, and B.V. McKoy.
- "Photoexcitation and Ionization in Molecular Fluorine: Stieltjes-Tchebycheff Calculations in the Static-Exchange Approximation," *The Journal of Chemical Physics* **72**, 1265 (1980), with A.E. Orel, T.N. Rescigno, and B.V. McKoy.
- "Theoretical Studies of Partial-Channel Cross Sections in Diatomic and Polyatomic Molecules," *Journal de Chimie Physique* **77**, 590 (1980), with N. Padial, G. Csanak, T.N. Rescigno, and B.V. McKoy.
- "Theoretical Studies of Photoionization in Diatomic and Polyatomic Molecules," *International Journal of Quantum Chemistry* **S14**, 285 (1980), with N. Padial, G. Csanak, T.N. Rescigno, and B.V. McKoy.
- "Photoexcitation and Ionization in Ozone: Stieltjes-Tchebycheff Studies in the Separated-Channel Static-Exchange Approximation," *The Journal of Chemical Physics* **74**, 4581 (1981), with N. Padial, G. Csanak, and B.V. McKoy.
- "Photoexcitation and Ionization in Carbon Dioxide: Theoretical Studies in the Separated-Channel Static-Exchange Approximation," *The Physical Review A* **23**, 218 (1981), with N. Padial, G. Csanak, and B.V. McKoy.
- "Theoretical Studies of Inner-Valence-Shell Photoionization Cross Sections in N₂ and CO," *Chemical Physics* **58**, 71 (1981), with S.R. Langhoff, T.N. Rescigno, J. Schirmer, L.S. Cederbaum, W. Domcke, and W. von Niessen.
- "Extended-Basis-Set RPAE Calculations of Molecular Photoionization Cross Sections: Theoretical Studies of Channel Coupling in N₂ and CO," *Chemical Physics Letters* **78**, 21 (1981), with G.R.J. Williams.
- "Experimental and Theoretical Studies of the Valence-Shell Photoionization Cross Sections of Acetylene: Strong Autoionization in the $(1\pi^{-1})^2\Pi$ Partial Channel," *Chemical Physics Letters* **83**, 270 (1981), with B.V. McKoy, R. Unwin, and A.M. Bradshaw.
- "Stieltjes Orbitals for Molecular Photoionization Continua," *Chemical Physics Letters* **82**, 242 (1981), with M.R. Hermann.
- "Theoretical Studies of Photoexcitation and Ionization in H₂O," *The Journal of Chemical Physics* **76**, 1043 (1982), with G.H.F. Diercksen, W.P. Kraemer, T.N. Rescigno, C.F. Bender, B.V. McKoy, and S.R. Langhoff.
- "Photoexcitation and Ionization in Acetylene," *The Journal of Electron Spectroscopy and Related Phenomena* **25**, 1 (1982), with L.E. Machado, E.P. Leal, G. Csanak, and B.V. McKoy.
- "Experimental and Theoretical Studies of the Valence-Shell Dipole Excitation Spectrum of Molecular Fluorine," *Chemical Physics* **66**, 435 (1982), with A.P. Hitchcock, C.E. Brion, and G.R.J. Williams.

- “Aspects of Molecular Photoionization,” *Journal of Molecular Science* (Wuhan, China) **2**, 15 (1982).
- ”Aspects of Electronic Configuration Interaction in Molecular Photoionization,” in *Electron-Atom and Electron-Molecule Collisions*, edited by J. Hinze (Plenum, New York, 1983), pp. 297-314.
- ”Löwdin Partitioning in a Lanczos Basis: Applications to Scattering States,” *International Journal of Quantum Chemistry* **23**, 135 (1983), with M.R. Hermann.
- ”Schrödinger Spectra,” in *Computational Molecular Physics*, edited by G.H.F. Diercksen and S. Wilson (Reidel, Dordrecht, Holland, 1983) pp. 299-334.
- ”Explicit Hilbert-Space Representations of Schrödinger States: Definitions and Properties of Stieltjes-Tchebycheff Orbitals,” *The Journal of Mathematical Physics* **24**, 541 (1983), with M.R. Hermann.
- ”Explicit Hilbert-Space Representations of Atomic and Molecular Photoabsorption Spectra; Computational Studies of Stieltjes-Tchebycheff Functions,” *The Physical Review A* **28**, 1957 (1983), with M.R. Hermann.
- ”Computational Studies of First-Born Scattering Cross Sections: I. Spectral Properties of Bethe Surfaces,” *The Journal of Computational Physics* **49**, 44 (1983), with D.J. Margoliash.
- ”Computational Studies of First-Born Scattering Cross Sections: II. Moment-Theory Approach,” *The Journal of Computational Physics* **49**, 67 (1983), with D.J. Margoliash.
- ”Experimental and Theoretical Studies of the Valence Shell Dipole Excitation Spectrum of HF,” *Chemical Physics* **88**, 65 (1984), with A.P. Hitchcock, G.R.J. Williams, and C.E. Brion.
- ”Stieltjes Orbitals for Molecular Photoexcitation and Ionization Spectra: $N \rightarrow V_\sigma$ and $N \rightarrow V_\sigma$ Resonance Features in CO and H₂CO Cross Sections,” *International Journal of Quantum Chemistry* **18**, 719 (1984), with M.R. Hermann, G.H.F. Diercksen, and B.W. Fatyga.
- ”Theoretical Studies of Photoionization of Nitric Oxide: Multiplet-Specific Shapes of $(5\sigma^{-1})b^3\Pi$ and $(5\sigma^{-1})A^1\Pi$ Partial Cross Sections,” *Chemical Physics Letters* **109**, 150 (1984), with M.R. Hermann and S.R. Langhoff.
- ”Molecular Photoionization Resonances: A Theoretical Chemist’s Perspective,” in *Resonances in Electron-Molecule Scattering, van der Waals Complexes, and Reactive Chemical Dynamics*, edited by D.G. Truhlar (American Chemical Society, Washington, D.C., 1984), pp. 113-138.
- ”Molecular Photoionization Processes of Astrophysical Interest,” in *Molecular Astrophysics*, edited by G.H.F. Diercksen, W. Huebner, and P.W. Langhoff (Reidel, Dordrecht, Holland, 1985), pp. 551-573.
- ”Preface to the Workshop,” in *Molecular Astrophysics*, edited by G.H.F. Diercksen, W. Huebner, and P.W. Langhoff (Reidel, Dordrecht, Holland, 1985), pp. xiii-xxiii, with G.H.F. Diercksen and W. Huebner.
- ”Valence-Shell Momentum Distributions and Ionization Energies of Carbon Disulfide,” *Chemical Physics* **96**, 227 (1985), with K.T. Leung, C.E. Brion, and B.W. Fatyga.

"Photoionization of Carbon Disulfide: Theoretical Studies of Outer- Valence-Shell Partial Cross Sections," *Chemical Physics Letters* **123**, 345 (1986), with B.W. Fatyga, M.R. Hermann, and G.H.F. Diercksen.

"Theoretical Studies of Photoionization in Nitric Oxide: Multiplet-Specific Effects in Vibrationally Resolved $5\sigma^{-1}$ Resonant Channels," *Chemical Physics Letters* **125**, 336 (1986), with M.R. Hermann, S.R. Langhoff, and T.J. Gil.

"Theoretical Studies of Valence-Shell Photoexcitation and Ionization Cross Sections in Nitric Oxide," *Chemical Physics* **109**, 1 (1986), with M.R. Hermann, C.W. Bauschlicher, W. Huo, and S.R. Langhoff.

"Theoretical Studies of Photoexcitation and Ionization in Hydrogen Sulfide," *Chemical Physics* **112**, 227 (1987), with G.H.F. Diercksen.

"Photoionization of Carbonyl Sulfide: Threshold Resonance Features in Outer-Valence-Shell Partial Cross Sections," *Chemical Physics Letters* **135**, 109 (1987), with J.A. Sheehy.

"Polarized Fluorescence Spectroscopy of O_2^+ ," *The Journal of Chemical Physics* **87**, 3299 (1987), with J.W. Keller, W.T. Hill, III, D.L. Ederer, and T.J. Gil.

"Polarization of X-Rays Fluorescence," *Physical Review Letters* **60**, 1010 (1988), with D.W. Lindle, P.L. Cowan, R.E. LaVilla, T. Jach, R.D. Deslattes, B. Karlin, J.A. Sheehy, and T.J. Gil.

Numerical Multi-Configurational Hartree-Fock Studies of Atomic Photoionization Cross Sections: Dynamical Core-Polarization Effects in Atomic Sodium," *The Physical Review A* **38**, 1279 (1988), with H.P. Saha and C. Froese-Fischer.

"Hilbert-Space Formulation of Feshbach-Fano Methods for Atomic and Molecular Photoionization: Optimal Choice of Zeroth-Order States in Shape-Resonance Channels," *Chemical Physics Letters* **151**, 417 (1988), with C.L. Winstead.

"Stieltjes Methods for Schrödinger Spectra: Hilbert-Space Approximations to the Discrete and Continuum Eigenstates of Spatially Anisotropic Hamiltonian Operators," in *Mathematical Frontiers in Computational Chemical Physics*, D.G. Truhlar, Editor (Springer, Berlin, 1988), pp. 85-135.

"Absolute Cross Sections for Molecular Photoabsorption, Partial Photoionization, and Ionic Photofragmentation Processes," *Journal of Physical and Chemical Reference Data* **17**, 9-153 (1988), with J.W. Gallagher, C.E. Brion, and J.A.R. Samson.

"Photoionization," in *Report on the Workshop on New Directions in Soft X-Ray Near-Threshold Phenomena*, edited by D.W. Lindle and R.C.C. Perera (LBL-25545, National Technical Information Service, 1988), pp. 6-13.

"Vibrational Averaging Effects on the Valence-Shell Electron Momentum Distributions in H_2O Employing Hartree-Fock-Limit Wavefunctions," *Chemical Physics Letters* **157**, 135 (1989), with K.T. Leung and J.A. Sheehy.

"Correlation of Molecular Valence- and K-Shell Photoionization Resonances with Bond Lengths," *The Journal of Chemical Physics* **91**, 1796 (1989), with J.A. Sheehy, T.J. Gil, C.L. Winstead, and R.E. Farren.

"Lanczos Methods for Hamiltonian Spectra: Hilbert-Space Approximations to Interaction-Prepared States," *Computer Physics Communications* **53**, 123 (1989), with T.J. Gil and C.L. Winstead.

"New Theoretical Perspectives on Molecular Shape Resonances: Feshbach-Fano Methods for Mulliken-Orbital Analysis of Photoionization Continua, *Physica Scripta* **T31**, 179 (1990), with T.J. Gil, C.L. Winstead, J.A. Sheehy, and R.E. Farren.

"Theoretical Studies of Photoionization in C_2H_2 , C_2H_4 , and C_2H_6 : Correlation of Prominent Spectral Features with C-C and C-H Antibonding Orbitals," *Chemical Physics Letters* **177**, 307 (1991), with R.E. Farren and J.A. Sheehy.

"Feshbach-Fano Formalism in Hilbert Space: Applications to Shape Resonances in Molecular Photoionization," *The Journal of Chemical Physics* **95**, 3107 (1991), with C. Winstead.

"Absorption and Emission Spectroscopy of High-Temperature Metal Vapors for Solar Thermal Propulsion," in *Proceedings of the 1993 JANNAF Propulsion Meeting* (Chemical Propulsion Information Agency, Johns Hopkins University, Columbia, 1993), Vol. 5. pp. 281-295, with C.W. Larson, M.E. Fajardo, P.G. Carrick, P.S. Erdman, W.C. Stwalley, and J.D. Mills.

"Solar Photochemical Hydrogen Bromide for Electrolytic Hydrogen Production," in *Proceedings of the Annual Review Meeting of the Department of Energy/Office of Utility Technology Hydrogen Program*, (Coral Gables, FL, 18-21 April 1995), with R.E. Schlieff, R.J. Hanrahan, and M. Stoy.

"Spectral Theory of Physical and Chemical Binding," *The Journal of Physical Chemistry* **100**, 2974 (1996).

"Resonant X-Ray Raman Scattering from Molecular K-Edges," in *Raman Emission by X-Ray Scattering*, D.L. Ederer and J.H. McGuire, Editors (World Scientific, Singapore, 1996), pp. 169-192, with J.D. Mills.

"X-Ray Raman Scattering from Molecular K-Edges," in *Atomic Physics with Hard X-Rays from High Brilliance Synchrotron Light Sources*, S. Southworth and D. Gemmel, Editors (Argonne National Laboratory Report ANL/APS/TM-16, Argonne IL, 1996), pp. 19-41, with J.D. Mills.

"Nondipole Resonant X-Ray Raman Spectroscopy: Polarized Inelastic Scattering at the K Edge of Cl_2 ," *Physical Review Letters* **79**, 383 (1997), with J.D. Mills, J.A. Sheehy, T.A. Ferrett, S.H. Southworth, R. Mayer and D.W. Lindle.

"Exciting Green Fluorescent Protein," in *Combined Quantum Mechanical and Molecular Mechanical Methods*, J. Gao and M.A. Thompson, Editors, ACS Symposium Series 712 (American Chemical Society, Washington, DC, 1998), Chapter 19, pp. 288-295, with V. Helms, E.F.Y. Hom, T.P. Straarsma, and J.A. McCammon.

"Reply to Comment on Nondipole Resonant X-Ray Raman Spectroscopy: Polarized Inelastic Scattering at the K Edge of Cl_2 ," *Physical Review Letters* **82**, 667 (1999), with J.D. Mills, J.A. Sheehy, T.A. Ferrett, S.H. Southworth, R. Mayer and D.W. Lindle.

"Shedding Light on the Dark and Weakly Fluorescent States of Green Fluorescent Proteins," *Proc. Natl. Acad. Sci.* **96**, 6177-6182 (1999), with W. Weber, V. Helms, and J.A. McCammon.

“Low-Lying Electronic Excitations of the Green Fluorescent Protein Chromophore,” *Journal of Molecular Structure: THEOCHEM* **506**, 179-189 (2000), with V. Helms and C.L. Winstead.

“Beyond the Dipole Approximation: Angular Distribution Effects in the 1s Photoemission from Small Molecules,” in *X-Ray and Inner-Shell Processes, X-99*, R.W. Dunford, et.al., Editors (American Institute of Physics, Melville, NY, 2000), pp. 156-162, with O. Hemmers, H. Wang, D.W. Lindle, P. Focke, I.A. Selin, J.D. Mills, and J.A. Sheehy.

“Angular Distributions of Molecular-Field and Spin-Orbit Split Core Levels of Sulfur 2p Photoionization in OCS,” *J. Phys. B* **33**, L51-L57 (2000), with K. Kukk, J.D. Bozek, N. Berrah, and J.A. Sheehy.

“High-Resolution Molecular Inner-Shell Electron Spectroscopies,” in *X-Ray and Inner-Shell Processes, X-99*, R.W. Dunford, et.al., Editors (American Institute of Physics, Melville, NY, 2000), pp. 188-204, with J.D. Bozek, N. Berrah, E. Kukk, T.D. Thomas, T.X. Carroll, L.J. Saethre, and J.A. Sheehy.

“New Insights into Molecular Structure and Dynamics Using Soft X-Ray Electron Spectroscopy,” in *The Physics of Electronic and Atomic Collisions*, Y. Itikawa, et.al., Editors (American Institute of Physics, Melville, NY, 2000), pp. 163-171, with E. Kukk, J.D. Bozek, T.D. Thomas, T.X. Carroll, L.J. Saethre, J.A. Sheehy, and N. Berrah.

“On the Angular Distributions of Molecular Photoelectrons: Dipole Cross Sections for Fixed-in-Space and Randomly Oriented Molecules,” *Chem. Phys. Lett.* **346**, 341-346 (2001), with J.C. Arce, J.A. Sheehy, O. Hemmers, H. Wang, P. Focke, I.A. Selin, and D.W. Lindle

“Chromophore Protonation States and the Proton Shuttle Mechanism in Green Fluorescent Protein: Inferences Drawn from Ab Initio Theoretical Studies of Chemical Structures and Vibrational Spectra,” *J. Phys. Chem. B* **105**, 2850-2857 (2001), with H.-Y. Yoo, J.A. Boatz, V. Helms, and J.A. McCammon.

“On the Angular Distributions of Electrons Photoejected from Fixed-in-Space and Randomly Oriented Molecules,” *J. Electron Spectro. & Relat. Phenom.* **114-116**, 23-32 (2001), with J.C. Arce, J.A. Sheehy, O. Hemmers, H. Wang, P. Focke, I.A. Selin, and D.W. Lindle.

“Large Nondipole Effects in the Angular Distributions of K-Shell Photoelectrons from Molecular N₂,” *Phys. Rev. Lett.* **87**, 273003 1-4 (2001), with O. Hemmers, H. Wang, P. Focke, I.A. Selin, D.W. Lindle, J.C. Arce, and J.A. Sheehy.

“Dynamical Theory of Molecular Photoionization: Electron Ejection Dynamics and Angular Distributions from Molecules Fixed in Space,” *J. Electron Spectro. & Relat. Phenom.* **123**, 117-132 (2002), with J.C. Arce and J.A. Sheehy.

“Spectral Theory of Chemical Bonding,” in *Low-Lying Potential Energy Surfaces*, M. Hoffmann and K.G. Dyall, Editors (American Chemical Society Publication, Washington, DC, 2002), Chapter 10, pp. 221-237, with J.A. Boatz, R.J. Hinde, and J.A. Sheehy.

“Nondipole Electron Angular Distributions from Fixed-in-Space Molecules,” *Phys. Rev. Lett.* **89**, 033002 1-4 (2002), with R. Guillemin, O. Hemmers, D.W. Lindle, E. Shigemasa, K. LeGuen, D. Ceolin, C. Miron, N. Leclercq, P. Morin, and M. Simon.

“Spectral Theory of the Chemical Bond,” *Chemical Physics Letters* **358**, 231 (2002), with R.J. Hinde, J.A. Boatz, and J.A. Sheehy.

“Multiphoton Ionization Spectroscopy of AlAr_N Clusters,” *J. Phys. Chem. A* **107**, 6948-6965 (2003), with J. M. Spotts, C. K. Wong, M. S. Johnson, M. Okumura, J. A. Boatz, J. Sheehy, R. J. Hinde.

“Applications of Löwdin’s Metric Matrix: Atomic Spectral Methods for Electronic Structure Calculations,” in *Fundamental World of Quantum Chemistry: A Tribute to the Memory of Per-Olov Löwdin*, edited by Erkki Brändas and Eugene S. Kryachko (Kluwer Academic, Dordrecht, 2004), Vol. 3, pp. 97-114, with R.J. Hinde, J.A. Boatz, and J.A. Sheehy.

“Atomic Spectral Methods for Molecular Electronic Structure Calculations,” *J. Chem. Phys.* **121**, 9323-9342 (2004), with R.J. Hinde, J.A. Boatz, and J.A. Sheehy.

“Spectral Properties of Minimal-Basis-Set Orbitals: Implications for Molecular Electronic Continuum States,” *Int. J. Quantum Chem.* **102**, 948-955 (2005), with C.L. Winstead.

“Comment on Fano Lineshapes Revisited: Symmetric Photoionization from Pure Continuum Excitation,” *Physical Review Letters* **94**, 229301 (2005), with J.W. Cooper, C.H. Green, A.F. Starace, and C.L. Winstead,

O. Hemmers, R. Guillemin, D. Rolles, A. Wolska, D.W. Lindle, E.P. Kanter, B. Krässig, S.H. Southworth, R. Wehlitz, B. Zimmermann, V. McKoy, and P.W. Langhoff, “Low-Energy Nondipole Effects in Molecular Nitrogen Valence-Shell Photoionization,” *Physical Review Letters* **97**, 103006 (2006).

P.W. Langhoff, R.J. Hinde, J.D. Mills, and J.A. Boatz, “Spectral-Product Methods for Molecular Electronic Structure Calculations,” *Theor. Chem. Accounts*, **120**, 199-213 (2008).

M. Ben-Nun, J.D. Mills, R.J. Hinde, C.L. Winstead, J.A. Boatz, G.A. Gallup, and P.W. Langhoff, “Atomic Spectral-Product Representations of Molecular Electronic Structure: Metric Matrices and Atomic-Product Compositions of Molecular Eigenstates,” *J. Phys. Chem.*, **113**, 7687-7697 (2009).

P.W. Langhoff, “Computational Implementation of Spectral Theory” SBIR Final Report, Air Force Research Laboratory, FA9300-09-C-2001 (March, 2012).

K. Rollin, M. Ben-Nun, J.D. Mills, J.A. Boatz, and P.W. Langhoff, “Covalent Atomic Rydberg State Representations of Charge Transfer Contributions to Molecular Electronic Eigenstates,” *J. Chem. Phys.* (to be published).

M. Ben-Nun, J.D. Mills, K. Rollin, R.J. Hinde, J.A. Boatz, G.A. Gallup, and P.W. Langhoff, “Atomic Spectral Methods for Molecular Electronic Structure Calculations: Exact Atomic-Pair Representation of Aggregate Hamiltonian Matrices,” *Phys. Rev.* (to be published).