

• PETER W. LANGHOFF •

• Home and Work Sites •

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• 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 Career Development Program in Pharmacology

• Professional Society Affiliations •

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

• Chronology of Primary Professional Appointments •

1999-present - Department of Pharmacology, University of California, La Jolla, CA - Senior Fellow
1996-present - San Diego Supercomputer Center, University of California, La Jolla, CA - Senior Fellow
1996-present - Air Force Research Laboratory, Edwards AFB, CA - Senior NRC Research Associate;
AFOSR University Resident Research Professor; Senior Scientific Consultant
1986-96 - Indiana University, Bloomington, IN - Professor of Chemistry
1985-86 - Florida State University, Tallahassee, FL - Professor of Chemistry;
Founding Faculty Associate, Supercomputer Computations Research Institute
1977-85 - Indiana University, Bloomington, IN - Chairman, Program in Chemical Physics
1975-76 - Joint Institute for Laboratory Astrophysics, National Bureau of Standards
and University of Colorado, Boulder, CO - JILA Visiting Fellow
1969-75 - Indiana University, Bloomington, IN - Assistant/Associate Professor of Chemistry
1967-69 - Harvard University, Cambridge, MA - Postdoctoral Fellow in Theoretical Chemistry
1965-67 - U.S. Army Missile Command, Huntsville, AL - Technical Intelligence Officer
1962-65 - Cornell Aeronautical Laboratory (Calspan, Inc.), Buffalo, NY - Research Physicist
1958-62 - University of Buffalo, Buffalo, NY - Instructor in Physics

• Invited Visiting and Consulting Appointments •

Harvard College Observatory (1971); Department of Chemistry, Stanford University (1975); Department of Aeronautics and Astronautics, Stanford University (1976); Lawrence Livermore National Laboratory (1977-82); NASA Ames Research Center (1978-79); Max Planck Institute for Physics and Astrophysics, Munich (1980-85); University of Sydney (1981); University of Paris (1981); University of British Columbia (1983); Institute for Theoretical Atomic and Molecular Physics, Harvard University (1989-90); Santa Barbara Institute for Theoretical Physics (1991); AF Phillips Laboratory, Edwards AFB (1991); Department of Aeronautics and Astronautics, Stanford University (1992).

• **Professional Experience** •

Senior Fellow, Department of Pharmacology, University of California, La Jolla, CA - Participates in collaborative research in pharmacology and biochemistry performed under the auspices of National Institutes of Health support, particularly in scientific studies of non-invasive fluorescent protein markers for *in vivo* diagnostics and determinations of biomolecular cellular and extra-cellular trafficking. Prepares manuscripts for publication in peer-reviewed scientific journals, and makes contributed and invited presentations at national and international professional society meetings. Interacts with faculty colleagues in the School of Medicine and in the Departments of Pharmacology and Chemistry & Biochemistry on aspects of theoretical biochemistry and non-invasive visible and x-ray imaging methodologies. Reviews scientific publications for professional journals and research grant proposals for funding agencies.

Senior Fellow, San Diego Supercomputer Center, University of California, La Jolla, CA - Performs theoretical studies of the interactions of x-ray and ultraviolet radiation with materials of potential Department of Energy interest in support of concomitant experiments at the UC Berkeley Advanced Light Source and the Argonne National Laboratory Advanced Photon Source. Develops novel methods for computational studies of the structures and properties of matter under the auspices of federal grants, and collaborates in the research activities of graduate students and postdoctoral fellows in the interactions of x-ray and ultraviolet radiation with matter at the Berkeley and Argonne sites. Prepares manuscripts for publication in peer-reviewed scientific journals and reviews scientific publications for professional journals and research grant proposals for funding agencies.

AFOSR University Resident Research Professor; Senior National Academy of Sciences Research Associate; 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 heavy-lift 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 for advanced-concept propulsion systems, including chemical, solar, and nuclear driven methodologies. Prepares annual reports, makes presentations at DoD-sponsored space-power and other technical meetings, and prepares manuscripts for publication in peer-reviewed technical journals.

Professor of Chemistry and Founding Faculty Associate, Supercomputer Computations Research Institute, Florida State University, Tallahassee, FL - Assisted in establishing and developing the Institute under Department of Energy and State of Florida sponsorship. Directed the Research Institute Planning and University Supercomputer Resources Allocation Committees, prepared technical reports and made oral presentations to DoE and State of Florida sponsors. Supervised the installation of a campus-wide ethernet and related digital communications system. Developed graduate research programs in supercomputer computations, helped to recruit graduate students, and supervised postdoctoral and graduate student research projects. Prepared manuscripts for publication in peer-reviewed scientific journals and reviewed scientific publications for professional journals and research grant proposals for government funding agencies.

Professor and Chairman, Program in Chemical Physics, Indiana University, Bloomington, IN - As Chair, held overall academic administrative and budgetary responsibility, organized graduate-student recruiting efforts, and directed development and coordination of academic curricula, standards, and seminar activity. Secured support from funding sources, and represented the program to deans and other university administrators. As Professor, lectured in and aided in the development of graduate and undergraduate courses in the physical sciences. Prepared 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 (DARPA, AFOSR, AFRL), the National Aeronautics and Space Administration, the North Atlantic Treaty Organization, the Research Corporation, the Proctor and Gamble Foundation, and other agencies. Supervised postdoctoral and graduate student research projects sponsored by federal and other funding agencies, and prepared manuscripts for publication in peer-reviewed scientific journals. Held academic committee assignments, including University Computing Requirements and Graduate School Ph.D. Standards. Helped 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 participated in defining workshops for establishment of the DoE-sponsored Berkeley Advanced Light Source.

• Career Narrative - Selected Aspects •

Peter Wolfgang Langhoff was born in New York City to parents of French and German origin. He attended the NYC primary and secondary public school systems, received the B.S. degree in applied physics from Hofstra University, and was granted the Ph.D. degree in theoretical physics by the State University of New York on basis of a theoretical study of atomic non-linear optical susceptibilities.

He was employed as a research physicist at Cornell Aeronautical Laboratory (Calspan, Inc.), where he performed theoretical and computational studies in the pure and applied sciences, particularly of atmospheric molecular photo-processes and electromagnetic scattering signatures. His analysis of the radar scattering cross sections of tumbling objects helped in devising an early remote-site satellite inspection system designed to identify nuclear warheads placed in Earth orbit.

He served in the military at the rank of Captain with the U.S. Army Missile Command, performing technical intelligence analysis, ballistic missile defense research, and studies of the physics and chemistry of ballistic vehicle atmospheric re-entry. His activities there aided in defining the Soviet threat required in design of the U.S. antiballistic missile system, for which work he received the Army Commendation Medal upon his discharge from active duty.

He held a two-year postdoctoral appointment at Harvard University in the Department of Chemistry. His joint publications with faculty colleagues there included a widely-cited review of aspects of the interactions between radiation and matter, and papers introducing Pade' approximant techniques in chemical physics, particularly for studies of optical properties and long-range interatomic interaction potentials. He held an adjunct appointment during this period at the MIT Lincoln Laboratory, continuing work in ballistic missile defense research, particularly on the chemistry of hypersonic re-entry vehicle wakes.

He joined the Faculty in Chemistry at Indiana University as Assistant Professor, was promoted to Associate Professor and to Professor, at which time he became Chairman of the Program in Chemical Physics. His research group at Indiana University was supported through the years by public- and private-sector funds, and graduated approximately twenty-five Ph.D. students under his supervision. He has published fifteen book chapters, approximately one hundred and fifty peer-reviewed scientific articles, and a large number of laboratory research reports on a wide range of topics in the pure and applied sciences.

During his tenure at Indiana University he also held continuing adjunct and related consulting appointments at the Lawrence Livermore Laboratory, the Max Planck Institute for Physics and Astrophysics, the NASA Ames Research Center, and, in the private sector, at Solar Reactor Technologies, Inc., as Vice President of Research and Technical Director. Additionally, he has collaborated widely and held visiting appointments of various durations at other institutions, including Stanford University, Harvard University, the University of British Columbia, the University of Paris, the University of Sydney, the Santa Barbara Institute for Theoretical Physics, the Harvard Institute for Theoretical Atomic and Molecular Physics, and the USAF Phillips Laboratory.

He has held nationally competitive fellowship awards including a Brandeis University NSF Summer Institute Fellowship in Physics, Senior National Research Council Postdoctoral Fellowships, AFOSR Phillips Laboratory Faculty Summer Research Fellowships, ASEE Stanford-Ames Summer Faculty Fellowships, an AFOSR University Resident Research Professorship, and, most recently, a National Institutes of Health Career Development Award.

His present research interests, pursued under the auspices of DoD, NSF, DoE, and NIH collaborative research grants, are centered on the interactions of uv and x-ray radiation with matter, on development of novel and efficient methods for predictions of the structures and properties of materials, and on protein science and the development of pharmacological diagnostic methods, particularly employing non-invasive fluorescent and other markers for *in vivo* studies of cell function, interaction, and pathologies. He holds appointments in the University of California, San Diego, Department of Pharmacology and the Department of Chemistry & Biochemistry, where his biomedically related studies are performed, and in the San Diego Supercomputer Center and the Air Force Research Laboratory, where his studies of the interactions of uv and x-ray radiation with matter and of the structures and properties of materials are performed.

• Recent Publications and Invited (I) & Contributed (C) Presentations •

J.W. Cooper, C.H. Green, P.W. Langhoff, A.F. Starace, and C.L. Winstead, "Comment on Fano Line-shapes 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.

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, and J.A. Sheehy, "Atomic Spectral Methods for Molecular Electronic Structure Calculations," *J. Chem. Phys.* **121**, 9323-9342 (2004).

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.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.

P.W. Langhoff, J.A. Boatz, R.J. Hinde, 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.

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).

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).

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 N_2 ," *Phys. Rev. Lett.* **87**, 273003 1-4 (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).

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).

K. Kukk, 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).

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.

"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).

"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).

"Spectral Theory of the Chemical Bond," *Proceedings of the High-Energy-Density-Matter Contractor's Conference*, Park City, UT, 25 October 2000 (I).

"Theory of Nonadditive N-Body Interactions in Atomic Clusters," March Meeting of the American Physical Society, Long Beach, CA, in *Bulletin of the American Physical Society* **43**, 27 (1998) (C).

• Pending Publications •

V.-A. Glezakou, J.A. Boatz, P.R. Taylor, J. A. McCammon, and P.W. Langhoff, "Ab Initio Theoretical Studies of Isotopic Substitutions in the Infra-Red and Raman Spectra of Green Fluorescent Protein Chromophores," *Journal of Physical Chemistry* (pending).

J.M. Spotts, C.K. Wong, M.S. Johnson, M. Okumura, J.A. Boatz, J.A. Sheehy, and P.W. Langhoff, "Experimental and Theoretical Characterization of the $X^2\Pi_{1/2}(3p) \rightarrow G^2\Sigma^+(4p)$ Bound-to-Continuum Transition in AlAr" *J. Chem. Phys.* (pending).

K. Greenwald, J.M. Maxwell, and P.W. Langhoff, "K-Edge Photoabsorption and Fragmentation Anisotropy in N₂ and O₂: Local-Hole and Lineshape Effects on Angular Distributions," *Chemical Physics Letters* (pending).

P.W. Langhoff, J.D. Mills and A. Dalgarno, "Resonance Raman Assisted Atomic Association: Application to Molecular Hydrogen Formation," *Astrophysics Letters* (in preparation).

P.W. Langhoff and D. Bershader, "Aspects of Dusty Shocks," *American Institute of Aeronautics and Astronautics Journal* (in preparation).

• **Comprehensive Publication List** •

Topical Areas of Publication: Atomic and Molecular Physics; Optical Physics, Dispersion, Scattering, Fluorescence; Mathematical and Theoretical Physics; Aeronautics, Astronautics, and Molecular Astrophysics; Molecular Photoionization and Photoabsorption Spectroscopy; Protein Structure and Properties; Quantum Chemistry; Classical and Quantum Molecular Dynamics Simulations of Matter.

Journals of Publication: 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, Journal of Physical Chemistry, Journal of Molecular Structure, Journal of Physics, 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, and American Institute of Aeronautics and Astronautics Journal.

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

"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 Rayleigh-Schrödinger and Green's-function Calculations of Ionization Potentials and Electron Affinities," *Chemical Physics Letters* 49, 421 (1977).

"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.

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

"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 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 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 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).
- "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* A23, 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.

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