PROFESSIONAL DATA ON DAVID A. MICHA

Born in Villa Mercedes (S. Luis), Argentina; U.S. citizen, 1974.

Education

- Lic. Phys. (M.Sc.), University of Cuyo, Bariloche, Arg., 1962
- Fil. Lic. (Ph.D.), University of Uppsala, Sweden, 1965
- Fil. Doktor (D.Sc.), University of Uppsala, Sweden, 1966

Professional Record

Appointments

- Research Associate, Quantum Chemistry Group, University of Uppsala, Sweden, November 1965-January 1966
- Research Associate, Theoretical Chemistry Institute, University of Wisconsin, Madison, May 1966-July 1967
- Assistant Research Physicist, Institute for Pure and Applied Physical Sciences and Department of Physics, University of California, San Diego (La Jolla), August 1967-August 1969
- Associate Professor of Chemistry and Physics, University of Florida, Gainesville, September 1969-June 1974
- Professor of Chemistry and Physics, University of Florida, Gainesville, July 1974-present

Visiting Positions

- Visiting Research Associate, Department of Physics, University of Buenos Aires, Argentina, March-April 1966
- Visiting Lamberg Professor, Institute of Physical Chemistry, University of Gothenburg, Sweden, July-December 1970
- Visiting Professor, Department of Chemistry and College Observatory, Harvard University, Cambridge, Massachusetts, September-December 1972
- Visiting Professor, Institute for Pure and Applied Physical Sciences, University of California, San Diego, July-September 1973
- A. Von Humboldt Senior Scientist Awardee, Max-Planck Inst. fur Strömungsforschung, Göttingen, West Germany, July-December 1976

- Visiting Professor, Quantum Chemistry Department, Uppsala University, Sweden, January-April 1977
- Visiting Professor, Physics Department, Imperial College, London, England, April-July 1977
- Visiting Scientist, Max-Planck Inst. fur Strömungsforschung, Göttingen, West Germany, September 1980
- Visiting Research Physicist, Institute of Theoretical Physics, University of California, Santa Barbara, August-November 1982
- Visiting Fellow, JILA and University of Colorado, Boulder, January-June 1983
- Visiting Professor, Weizmann Institute of Science, Rehovot, Israel, July-September 1983
- Faculty Research Participant, Oak Ridge National Laboratory, June-July 1984
- Visiting Scientist, Quantum Chemistry Department, Uppsala University, July-August 1986
- Visiting Professor, University of Buenos Aires, Argentina, May 1988, and May, 1995.
- Visiting Scientist, Institute for Theoretical Atomic and Molecular Physics, Harvard University, August-December, 1990.
- Visiting Scientist, Chemistry Department and Supercomputer Computations Research Institute, Florida State University, January-May, 1991.
- A. von Humboldt Foundation Visiting Professor, Max Planck Institute fur Astrophysik, Munich, and Max Planck Institute fur Stroemungsforschung, Goettingen, Germany, May-July, 1996, and May-June, 1997.
- Visiting Scientist Fellowship, Institute for Theoretical Atomic and Molecular Physics, Harvard University- Smithsonian Center for Astrophysics, June-August 1998; April-July 2000.

Membership in Professional Societies

- American Physical Society
- American Chemical Society
- Sigma Xi Scientific Society

Membership in Honorary Societies, Honors and Awards.

- Fellowship, Swedish International Development Agency, 1962-65

- Member, Society of the Sigma Xi, 1966
- Docent, University of Uppsala, 1968
- Fellow, Alfred P. Sloan Foundation, 1971-74
- Visiting Lamberg Professor, University of Gothenburg, 1971
- U.S. Senior Scientist Award, A. Von Humboldt Foundation, W. Germany, 1976; re-invited in 1996
- Fellow, American Physical Society, 1976
- J.I.L.A. Fellow, National Bureau of Standards, 1983
- Sigma Xi Senior Faculty Research Award, University of Florida, 1985
- Listed in "American Men and Women of Science" (Reed Publ. Co, 1992) and following ones.
- Listed in "Who-is-Who in Science and Engineering", 2nd edition (Marquis, 1993) and following ones.
- Listed in "Who-is-Who in America", 49th edition (Marquis, 1995) and following ones.
- University of Florida Teaching Award, 1996-97
- University of Florida Award to Outstanding Faculty, 1999.

Research Grants

- Principal Investigator, American Chemical Society - Petroleum Research Fund, Grant, 1969-72
- Principal Investigator, National Science Foundation Grant, 1971-73
- Alfred P. Sloan Fellowship, 1971-73; extended to 1973-75
- Travel Grant, National Research Council - National Science Foundation, 1971
- Principal Investigator, National Science Foundation Grant, 1973-75
- Division of Sponsored Research, Travel Support, 1974
- Principal Investigator, National Science Foundation Grant, 1975
- Principal Investigator, National Science Foundation Grant, 1976-77
- Travel Grant, National Research Council - National Science Foundation, 1975
- NATO Research Collaboration Grant, 1976-82
- Oak Ridge Participation Contract, 1977-present
- Principal Investigator, National Science Foundation Grant, 1977-80
- National Resource for Computation in Chemistry, 1978-80
- A. Von Humboldt Foundation Award, 1976-77
- National Science Foundation Supplement, 1979
- National Science Foundation U.S.-Latin American Coop. Science Program, 1979
- National Science Foundation, Sanibel Symposium Support, 1979
- National Resource for Computation in Chemistry, Sanibel Symposium Support, 1979
- Division of Sponsored Research, University of Florida, 1979
- Division of Sponsored Research, University of Florida, Faculty Award, 1980
- Principal Investigator, National Science Foundation, 1980-83
- Principal Co-Investigator, NASA, 1981-82
- Principal Co-Investigator, NASA, 1982

- Office of Naval Research, Bates International Symposium Support, 1983
- Principal Co-Investigator, NASA, 1983
- Principal Investigator, Air Force Office of Scientific Research, Bates International Symposium Support, 1983
- Principal Investigator, NSF, 1984-86
- Principal co-investigator, NATO Research Collaboration Grant, 1985-86
- Principal co-investigator, NSF International Program, USA-Yugoslavia, 1986-89
- Swedish National Science Research Council Grant, 1986
- Principal Investigator, NSF, 1987-89
- Principal Investigator, Office of Naval Research, 1987
- Principal co-investigator, NSF International Program, USA-Argentina, 1988-90
- Principal Investigator, UF Division of Sponsored Research
- Principal Investigator, NSF, 1990-92
- Principal Investigator, Florida Space Research Consortium (NASA), 1990-91.
- Principal Investigator, UF Division of Sponsored Research, 1991
- Principal co-investigator, NSF International Program, USA-Yugoslavia, 1991-92
- Principal Investigator, UF Division of Sponsored Research, 1992
- Principal Investigator, UF Division of Sponsored Research, 1993 (two awards).
- Principal Investigator, NSF Chemistry Division, 1993-96
- Principal Co-Investigator, Office of Naval Research Chemistry Division, 1993-94
- Principal Investigator, Office of Naval Research Physics Division, 1993-94 (US-LA Workshop)
- Principal Investigator, NSF International Programs Division, 1993-94
- Principal Co-Investigator, Office of Naval Research Chemistry Division, 1995-96, 1997-98.

- Principal Investigator, Office of Naval Research Physics Division, 1996-97 (US-LA Workshop)
- Principal Investigator, NSF Chemistry Division, 1997-99
- Principal Investigator, Office of Naval Research Physics Division, 1999 (US-LA-C-C Workshop)
- Principal Co-Investigator, Office of Naval Research Chemistry Division, 1998-2000.
- Principal Investigator, NSF Chemistry Division, 1999-2002
- Principal Investigator, Office of Naval Research Physics Division, 2001 (Pan-American Workshop)
- Principal Investigator, NSF Chemistry Division, 2003-2005
- Principal Investigator, Office of Naval Research Physics Division, 2003 (Pan-American Workshop)
- Principal Investigator, NSF Chemistry Division, 2006-2009

Present Research Interests

- Energy transfer, electron transfer, and reactions in gas phase collisions
- Energy and electron transfer at solid surfaces
- Molecular photodissociation, and photodesorption from surfaces
- Dynamics of atomic clusters
- Intermolecular forces
- Quantum molecular dynamics
- Few- and many-body theory of atomic collisions
- Density matrix theory of extended molecular systems
- Time-dependent molecular orbital and many-electron theory
- Computational methods of molecular scattering, dynamics, and electronic structure
- Visualization and animation of molecular interactions
- Physical models of quantum computers

Departmental Activities, University of Florida

- Member of the Quantum Theory Project, 1969-present
- Committee on Colloquium Speakers for the 1970-71 Academic Year, Department of Chemistry
- Committee on Award for Best Presentation in Physical Chemistry, American Chemical Society Local Meeting, 1971
- Committee on Postdoctoral Applicants, Department of Chemistry, 1972-73
- Search Committee for New Assistant Professors, 1973-75
- Committee for Selection of New Graduate Students, Department of Chemistry, 1973-80, 1984-2000
- Committee on Colloquium Speakers, Department of Chemistry, 1974-75
- Chairman, Departmental Seminar Committee, Department of Chemistry, 1979-81
- Graduate Advisory and Curriculum Committee, Department of Chemistry, 1980-83
- Space Committee, Department of Chemistry, 1980-83
- Language Committee, Department of Chemistry, 1983-92
- Undergraduate Student Advisory Committee, Department of Chemistry, 1983-92
- Faculty Recruiting Committee, Department of Chemistry, 1988
- Graduate Recruiting and Curriculum Committee, Department of Chemistry, 1985-2000
- Chairman, Faculty Recruiting Committee, Department of Chemistry, 1989
- Physical Chemistry Committee, PhD written qualifying exams, 1993, 1996
- Technical Facilities Committee, 1994-2000
- Chairman, Instruction Committee, 1997-2000
- Acting Head, Physical Chemistry Division, 1999-2000
- Head, Physical Chemistry Division, 2000-2005

College, Graduate School, and University of Florida Activities

- Member of the Quantum Theory Project, 1969-present
- University Committee for Selection of Fullbright-Hays Fellows, 1974
- Division of Sponsored Research Committee for University Funding of Projects, 1974
- Assistant Director of Quantum Theory Project (computer budget, library acquisitions), 1973-74
- Committee Member, Chemical Physics Program of the Graduate School, 1977-82
- College of Arts and Sciences Committee for Allocation of Computing Funds, 1978-80
- Council for International Studies, Graduate School, 1979-83
- Associate Director, Sanibel Symposium on the Quantum Theory of Matter, March 12-18, Palm Coast, Florida (also, Session Chairman), 1979
- Co-Organizer, Symposium on the Quantum Theory of Matter, March 9-14, Palm Coast, Florida (also, Session Chairman), 1981
- Deputy Director, Symposium on the Quantum Theory of Matter, March 7-13, Palm Coast, Florida, 1982
- Associate Director, Quantum Theory Project, 1982
- Co-organizer, Bates International Symposium, March 3-5, Palm Coast, Florida, 1983 (also, organizer of the scientific program and editor of its proceedings)
- Proposal Review Committee, Division of Sponsored Research, University of Florida, 1983-84
- Organizing Committee, "Sanibel Symposia," Florida, 1984-present
- Director, Center for Chemical Physics, 1982-91
- Committee Member, Center for Chemical Physics, 1992-2000; member 2000-present
- Organizer, UF-FSU Exchange Program on Advanced Scientific Computing, 1991-97
- Organizer, US-Latin American Workshop on Molecular and Materials Sciences, UF, 1993, 1994, 1997, 1999.
- Member, University Senate, 1997-99
- Member, UF Minority Mentors Program, 1994-98.

- Member elected by UF Senate, University Personnel Board, 1998
- Organizer, Pan-American Workshop on Molecular and Materials Sciences: Theoretical and Computational Aspects, UF, 2001.
- College of Liberal Arts and Sciences Tenure and Promotion Committee, 2006-2007

Professional Activities

- Assistant Editor, Proceedings of the International Symposium on Quantum Theory, Sanibel Island, 1971 (Wiley, New York, 1971).
- Local Committee, 24th Annual Gaseous Electronics Conference and 3rd Arc Symposium, American Physical Society, Gainesville, 1971.
- Chairman, Session on "Radiative Lifetimes," 24th Annual Gaseous Electronics Conference and 3rd Arc Symposium, American Physical Society, Gainesville, 1971.
- Leader, Session on "Scattering Problems," Quantum Theory Workshop, Sanibel Island, Florida, 1972 and 1973.
- Discussion Panel Member on "Molecular Problems," International Symposium on Quantum Theory, Sanibel Island, Florida, 1972.
- Consultant to U.S. Army, 1972-74, 1975-76.
- Chairman, "Atomic and Molecular Collisions" Session, American Physical Society March Meeting, San Diego, California, 1973.
- Chairman, Workshop on Molecular Collisions, V Southeast Theoretical Chemical Association, Tuscaloosa, Alabama, June 1974.
- Chairman, Workshop on Reactive Molecular Collisions, VII Southeast Theoretical Chemical Association, Tuscaloosa, Alabama, May 1976.
- Chairman of Session in European Conference on Molecular Low Energy Collisions, Trento, Italy, June 1976.
- International Advisory Committee, IX International Conference on Few-Body Problems in Physics and Chemistry, Eugene, Oregon, August 17-23, 1980, (1979-80).
- Session Chairman, X Southeast Theoretical Chemical Association Conference, Florida State University, Tallahassee, Florida, May 25, 1979.
- Co-organizer of the Palm Coast Symposium on the Quantum Theory of Matter, Palm Coast, Florida, March 12-18, 1979.
- Member of the Advisory Editorial Board, International Journal of Quantum Chemistry, 1979-1988.

- Reviewer, Canada National Research Council, 1982-present.
- Reviewer, National Science Foundation Programs in Chemical Physics, Chemical Instrumentation, Atomic Physics, International Programs, U.S.-Israel Binational Program, 1982-present.
- Reviewer, American Chemical Society Petroleum Research Fund, 1982, 1983.
- Referee, Journal of Chemical Physics, Journal of Physical Chemistry, International Journal of Quantum Chemistry, Physical Review A, Journal of Physics B, 1982-present.
- Special Editor, Proceedings of the International Symposium on the Quantum Theory of Matter, Palm Coast, Florida, March 3-12, 1983.
- Organizing Committee, "Sanibel International Symposia," Florida, 1984-present
- Organizing Committee Member, Conference on Few-Body Methods, Guang-Xi, P.R. China, Summer 1985.
- Member, Editorial Board, "Few-Body Systems" (Acta Physica Austriaca), 1985-present.
- Vice-chairman, American Physical Society Topical Group on Few-body Systems and Multiparticle Dynamics, 1986-88.
- Chairman, American Physical Society Topical Group on Few-body Systems and Multiparticle Dynamics, 1988-89.
- Member, Advisory Panel, NSF Division of Advanced Computational Sciences, 1990-92.
- Editor, Plenum Publishing Corp. Book Series on "Finite Systems and Multiparticle Dynamics", 1990-present.
- Member, Advisory Panel, NSF Program on Presidential Young Investigators Awards, March 1993
- Member, NSF review panel on Graduate Research Traineeships focusing on "Integration High Performance Computing into Research", November 1993.
- Member, International Advisory Committee, XIV Conference on Few-Body Problems in Physics, Williamsburg, Virginia, May 1994.
- Co-organizer, Division of Chemical Physics Program, 2 sessions on "Localized Phenomena in Extended Molecular Systems and at Interfaces" American Physical Society April 1994 meeting, Crystal City, Virginia

- Member, Dep. of Energy review panel, on "Large Computational Projects" of the Office of Enegy Research, June, 1994.
- Member, Nomination Committee, American Physical Society Topical Group on Few-body Systems and Multiparticle Dynamics, 1994.
- Organizer, "US-Latin American Workshop on Theoretical and Computational Aspects of Molecular and Materials Sciences", Univ. of Florida, 1993, 1994, 1997.
- Appointed member of the external advisory board of Clark-Atlanta University NSF Center for Theoretical Studies of Physical Systems, 1998.
- Co-organizer (with C. Harris, UC Berkeley) Amer. Physical Soc. Division of Chemical Physics Symposium on "Femtosecond Dynamics at Surfaces: Theory and Experiment", APS National March Meeting 1998.
- Co-organizer, "US-Latin America-Canada-Caribbean Workshop on Theoretical and Computational Aspects of Molecular and Materials Sciences", Cuernavaca, Mexico, 1999.
- Co-organizer, "Pan-American Workshop on Theoretical and Computational Aspects of Molecular and Materials Sciences", Gainesville FL, February 2001.
- Co-organizer (with J. Tully and U. Wille) "Atomic, Molecular and Optical Physics at Surfaces" ITAMP Workshop, Harvard-Smithsonian Center for Astrophysics, Cambridge MA, June 2001.
- Co-organizer, "2003 Pan-American Workshop on Theoretical and Computational Aspects of Molecular and Materials Sciences", Cuernavaca, Mexico.
- Co-organizer, Workshop on "Quantum Dynamics of Complex Molecular Systems", Paris Research Center, Paris (France) May 2005.
- Co-organizer, "2007 Pan-American Workshop on Theoretical and Computational Aspects of Molecular and Materials Sciences", Cuernavaca, Mexico, October 2007.
- Co-organizer, Workshop on "Quantum Dynamics of Complex Molecular Systems: Energy Flow Dynamics in Biomaterial Systems", Paris Research Center, Paris (France) October 2007
- Co-organizer, Workshop on " Coherence, Control, and Dissipation" Annual Program on Mathematics and Chemistry, Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, MN, 2008-09.

Supervision of Doctoral Dissertations

(Directed at the University of Florida)

1. Michael J. Redmon, Ph.D., Chemistry, 1973, "Dynamics of Alkali Atom-Halogen Atom Collisions"
2. John C. Bellum, Ph.D., Physics, 1976, "Electronic and Dynamic Aspects of Diatomic Systems"
3. Zeki C. Kuruoglu, Ph.D., Chemistry, 1978, "Three-Body Theory and Computational Aspects of Collisions between Atoms and Diatomic Molecules"
4. Lyntis H. Beard, Jr., Ph.D., Chemistry, 1979, "Energy Transfer and Dissociation in Hyperthermal Atom-Diatom Collisions"
5. Larry R. Relyea, Ph.D., Chemistry, 1980, "Theory of Ionizing Atomic Collisions at Thermal Energy"
6. Eduardo F. Vilallonga, Ph.D., Physics, 1981, "Energy Transfer in Molecular Collisions"
7. John A. Olson, Ph.D., Chemistry, 1982, "Dynamics of Diabatic Atom-Diatom Reactions at Low Energies"
8. Cliff D. Stodden, Ph.D., Chemistry, 1987, "Photodissociation of Polyatomic Molecules; State-to-State Cross Sections from the Selfconsistent Eikonal Method"
9. Zaida Parra-Gonzalez, Ph.D., Chemistry, 1988, "Scattering of Atoms by Solid Surfaces and by Adsorbates"
10. D. Srivastava, Ph.D. Physics, 1988, "Photoexcitation of Polyatomic Systems"
11. Joel M. Cohen, M.Sc., Chemistry, 1988, "Computational Studies of Molecular Collisions"
12. Joel M. Cohen, Ph.D. , Chemistry, 1990, "Computational Aspects of Electronically Diabatic Molecular Collisions"
13. Q. Feng, Ph.D. , Physics, 1991, "A Time-Dependent Molecular Orbital Approach to Ion- Solid Surface Collisions"
14. Keith Runge, Ph.D. Physics, 1993, "Time-Dependent Many-Electron Theory of Atomic Interactions"
15. Dario Beksic, Ph.D., Physics, 1994, "Electronically Diabatic Photodesorption of Molecules Adsorbed on Metal Surfaces"
16. Robert Asher, Ph.D., Chemistry, 1995 (D. A. M. and P. Brucat co-chairs), "Experimental and Theoretical Investigation and Characterization of Small Molecular Ions".

17. Herbert da Costa, Ph. D., Chemistry, 1998, "Time-Dependence of Light Emission and Spin-Orbit Coupling in Slow Atom-Atom Collisions".

18. Zhigang Yi, Ph. D., Physics, 1998, "Computational Aspects of the Quantum Molecular Dynamics of Adsorbates"

19. Andres Reyes, Ph. D., Chemistry, 2003, "Density Matrix Theory and Computational Aspects of Atomic Collisions Including Spin-Orbit Coupling"

20. Alberto Santana, Ph. D., Chemistry, 2003, "Photoinduced Quantum Dynamics of Adsorbates at Surfaces"

21. Brian Thorndyke, Ph. D., Physics, 2004 "Quantum Dynamics of Finite Atomic and Molecular Systems Through Density Matrix Methods"

22. Alexander Pacheco, Ph. D., Chemistry, 2006 "First Principles Dynamics of Transient Light Absorption and Emission of Alkali Atoms Interacting with Rare Gas Atoms"

23. Andrew Leathers, Ph. D. candidate, Chemistry

Teaching Activities

Graduate courses

- Chemical Bonding and Spectra, Part I, Graduate Course, Department of Chemistry, University of Florida, 1969, 1971 (Spring and Fall Terms), 1974, 1978, 1980, 1982, 1985, 1988, 1991, 1993, 1994.

- Statistical Thermodynamics, Graduate Course, Department of Chemistry, University of Florida, 1970, 1973, 1974, 1975, 1989, 1993, 1997, 1999, 2002, 2004, 2006.

- Chemical Physics (Alternates Intermolecular Forces, Molecular Scattering, Surface Science, Molecular Dynamics and Kinetics, Computational Methods), Graduate Course, Departments of Chemistry and Physics, University of Florida, Gainesville, 1972, 1973, 1975, 1976, 1978, 1979, 1981, 1983, 1985, 1988, 1990, 1992, 1996, 1998, 2001,2003, 2005, 2007.

- Chemical Bonding and Spectra, Part II, Graduate Course, Department of Chemistry, University of Florida, 1974, 1976, 1979, 1981.

- Kinetic Theory of Gases, Graduate Course, Department of Chemistry, University of Florida, Gainesville, 1976.

- Advanced Chemical Kinetics, graduate course, 1986, 1994.

- Chemical Thermodynamics, graduate course, 2003, 2004, 2005, 2006.

Undergraduate courses

- Physical Chemistry with Biological Applications, Department of Chemistry, University of Florida, Gainesville, 1972, 1973, 1975, 1978, 1980, 1984, 2004.

- Physical Chemistry, Part I, Undergraduate Majors Course, Department of Chemistry, University of Florida, Gainesville, 1978, 1980, 1984, 1992, 1993, 1995, 1996, 1997, 2000, 2004, 2005, 2006, 2007.

- Physical Chemistry II, Undergraduate Majors Course, Department of Chemistry, University of Florida, Gainesville, 1977, 1979, 1984, 1985, 1986, 1987, 1989, 1995, 1999, 2001, 2002,2003.

- General Chemistry I, Undergraduate Course, Department of Chemistry, University of Florida, Gainesville, 1981, 1998.

Institute and School courses

- Quantum Theory of Elementary Systems, Lecture Series, Winter Institute in Quantum Chemistry, Solid State Physics and Quantum Biology, University of Florida, Gainesville, 1969.

- Collision Theory, Lecture Series, Winter Institute, Sanibel Island, Florida, and International Summer Institute, Beistostolen, Norway, 1970.

- Molecular Collision Dynamics, Lecture Series, Graduate Level, Institute of Physical Chemistry, University of Gothenburg, Sweden, 1970.

- Introduction to Scattering Theory, Lecture Series, Winter Institute, University of Florida, Gainesville, 1972.

- Quantum Theory of Molecular Collisions, Lecture Series, I Latin American School of Theoretical Chemistry, Mexico, 1974.

- Intermolecular Forces, Lecture Series, I Latin American Advanced School on Theoretical Chemistry, University of La Plata, Argentina, 1981.

- Molecular Scattering Theory, Lecture Series, II Latin American Advanced School on Theoretical Chemistry, University of Montevideo, Uruguay, 1982.

- Introduction to Quantum Molecular Dynamics, Lecture Series, Winter Institute, Univ. of Florida, 1987, 1988.

- Theory of Molecular Photodissociation, Latin American School of Physics, Caracas, Venezuela, 1990.

- Lectures on "Quantum dynamics in an active medium: the example of femtosecond desorption", Gordon Summer School on Theoretical Chemical Physics, Bristol RI, June 22-23, 2000.

Publications

1. David A. Micha, "Degeneracy of Eigenvalues of Reduced Density Matrices and Time Reversal Invariance for Electron Systems," J. Chem. Phys. **41**, 3648-49 (1964).

2. David A. Micha, "Evolution of Molecular Systems and the Separation of Electronic and Nuclear Motions," J. Chem. Phys. **41**, 1947-51 (1964).

3. Frank E. Harris, David A. Micha and Herbert A. Pohl, "The Interaction Potential Surface of H_3," Arkiv for Fysik **30**, 259-66 (1965).

4. David A. Micha, "Quantum Mechanical Model for Simple Molecular Reactions," Arkiv for Fysik **30**, 411-23 (1965).

5. David A. Micha, "The Exchange Reaction of H and H_2," Arkiv for Fysik **30**, 425-36 (1965).

6. David A. Micha, "Angular Distribution of Products of Hydrogen Atom-Hydrogen Molecular Reactions," Arkiv for Fysik **30**, 437-47 (1965).

7. David A. Micha, "Molecular Reactions. A Study of Electronic and Collision Aspects of Exchange Molecular Reactions, with Applications to the Hydrogen Atom-Hydrogen Molecule System," Thesis, University of Uppsala, (Almqvist & Wiksells Boktrykeri AB, Uppsala, 1965).

8. David A. Micha, "Expansion of the T Matrix for Resonance Collisions," J. Math Phys. **8**, 1716-19 (1967).

9. David A. Micha, "Perturbation of Angular Correlations by Randomly Oriented, Fluctuation Magnetic Fields," Phys. Rev. **156**, 627-30 (1967).

10. David A. Micha, "Compound State Resonances in Molecular Collisions: The Integral Elastic Cross Section for D_2-Xe Scattering," Chem. Phys. Letters **1**, 139-42 (1967).

11. David A. Micha, "Compound State Resonances in Atom-Diatomic Molecule Collisions," Phys. Rev. **162**, 88-97 (1967).

12. David A. Micha, "Communication on Quantum Mechanical Calculations of Reactive Molecular Collisions," Discussions of the Faraday Society **44**, 77-78 (1967).

13. David A. Micha, "Exchange Effects in the Degenerate Perturbation Theory of Intermolecular Potentials," J. Chem. Phys. **48**, 3639-44 (1968).

14. David A. Micha, "Optical Potentials in Molecular Collisions," Invited paper to the Symposium of the Division of Chemical Physics (APS 1968 March Meeting, Berkeley, California) J. Chem. Phys. **50**, 722-26 (1969).

15. R. Marriott and David A. Micha, "Optical Potential for Li - HBr Collision at Low Energies," Phys. Rev. **180**, 120-23 (1969).

16. David A. Micha, "Many-Body Contributions to Atomic Correlation Energies," Phys. Rev. A **1**, 755-64 (1970).

17. David A. Micha and Manuel Rotenberg, "Impact Parameter Dependence of Vibrational Excitation Cross Sections for H_2 + He Collisions," Chem. Phys. Letters **6**, 79-82 (1970); idem 11, 626-27 (1971), (Addenda and Errata).

18. David A. Micha, S.Y. Tang and E.E. Muschlitz, Jr., "Semiempirical Model for Penning and Associative Ionization. Velocity Dependence and Branching Ratios for Ne* Collisions with Ar, Kr, and Xe," Chem. Phys. Letters **8**, 587-91 (1971).

19. David A. Micha and E. Brandas, "Variational Methods in the Wave-Operator Formalism. A Unified Treatment of Bound and Quasi-Bound Electronic and Molecular States," J. Chem. Phys. **55**, 4792-97 (1971).

20. David A. Micha, "Dynamics of Three Interacting Monovalent Atoms in the Faddeev Formalism," Proceedings of the VII International Conference Physic Electronics and Atomic Collisions, pp. 217-18 (North-Holland Publishing Co., Amsterdam, 1971).

21. Erkke Brandas and David A. Micha, "Variational Methods in the Wave Operator Formalism. Applications in Variation-Perturbation Theory and the Theory of Energy Bounds," J. Math. Phys. **13**, 155-60 (1972).

22. David A. Micha and M. Rotenberg, "Collision Energy Dependence of Angular Distributions for Vibrational Excitations of H_2 by He," Chem. Phys. Letters **13**, 289-91 (1972).

23. David A. Micha, "Collision Dynamics of Three Interacting Atoms: The Faddeev Equations," J. Chem. Phys. **57**, 2184-92 (1972).

24. Paul McGuire and David A. Micha, "Coupled-Channel Investigation of Rotationally and Vibrationally Inelastic Collisions between He and H_2," Int. J. Quantum Chem. **6**, 111-32 (1972).

25. Paul McGuire and David A. Micha, "Collision Dynamics of Three Interacting Atoms: Foundation of the Spectator-Stripping Model," Chem. Phys. Letters **17**, 207-10 (1972).

26. David A. Micha, "Long-Lived States in Atom-Molecule Collisions," Accounts Chem. Res. **6**, 138-44 (1973).

27. Paul McGuire and David A. Micha, "Dynamical Coupling in the Differential Equation Approach to Atom-Diatom Exchange Reactions," Molec. Phys. **25**, 1335-52 (1973).

28. Paul McGuire and David A. Micha, "Prediction of Spectator Stripping Dynamics for Exchange Reactions in T + H_3, T + D_2, and T + HD in the 10 eV Range," Proceedings VIII International Conference on Physic Electronics and Atomic Collisions, pp. 119-20 (Institute of Physics, Belgrad, Yugoslavia, 1973).

29. David A. Micha, "Effective Hamiltonian Methods for Molecular Collisions," Adv. Quantum Chem. **8**, 231-87 (1974).

30. David A. Micha, "Collision Dynamics of Three Interacting Atoms: Permutational Symmetry for Identical Nuclei," J. Chem. Phys. **60**, 2480-87 (1974).

31. John C. Bellum and David A. Micha, "A Study of Single-Electron and Total Energies for Some Pairs of Noble Gas Atoms," Intern. J. Quantum Chem., Symp. Proc. **8**, 229-40 (1974).

32. Michael J. Redmon and David A. Micha, "A Computational Method for Multi-Channel Scattering Calculations. Applications to Rotational Excitation and Long-Lived States of He-N_2," Chem. Phys. Letters **28**, 341-44 (1974).

33. Michael J. Redmon and David A. Micha, "Interaction Potentials and Dynamics for Li + F Collisions," Int. J. Quantum Chem., Symp. Proc. **8**, 253-62 (1974).

34. David A. Micha, "Recent Developments in the Theory of Reactive Molecular Collisions," Int. J. Quantum Chem., Symp. Proc. **8**, 263-68 (1974).

35. David A. Micha and Hiroki Nakamura, "Semi-Empirical Model for Angular Distribution of Electrons Emitted in Metastable Atom-Atom Collisions," Phys. Rev. A **11**, 1988-93 (1975).

36. David A. Micha, "Quantum Theory of Reactive Molecular Collisions," Adv. Chem. Phys. **30**, 7-75 (1975).

37. David A. Micha and Jian-Min Yuan, "Collision Dynamics of Three Interacting Atoms: The Multiple-Collision Expansion," J. Chem. Phys. **63**, 5462-69 (1975).

38. David A. Micha and Jian-Min Yuan, "Direct Atom-Diatomic Reactions by the Multiple-Collision Expansion: Application to Ar^+ + H_2 and K + I_2," Proc. IX International Conference on Physic Electronics and Atomic Collisions **1**, 589-90 (University of Washington Press, Seattle, 1975).

39. Jian-Min Yuan and David A. Micha, "Collision Dynamics of Three Interacting Atoms: Stripping Reactions of Ar^+ + H_2 and K + I_2," Chem. Phys. **64**, 1032-41 (1976).

40. David A. Micha, "Optical Models in Molecular Collision Theory," Chapter in Modern Theoretical Chemistry, Vol. IA: Dynamics of Molecular Collisions, W.H. Miller, ed., pp. 81-129 (Plenum Publ. Co., 1976).

41. Jian-Min Yuan and David A. Micha, "Collision Dynamics of Three Interaction Atoms: Electron Transfer in the Reactions of K + Br_2, BrI, and I_2," J. Chem. Phys. **65**, 4876-84 (1976).

42. David A. Micha, "Many-Body Theory of Molecular Collisions," in Methods and Structure of Quantum Science, J.-L. Calais, et al., editors (Plenum Publ. Co., 1976), pp. 367-80.

43. David A. Micha, "Operator Formalisms of Reactive Molecular Scattering," Int. J. Quantum Chem., Symp. Proc. **10**, 259-66 (1976).

44. David A. Micha, "Collision Dynamics of Three Interacting Atoms: A Method of Diatomics-in-Molecules," J. Chem. Phys. **66**, 1255-57 (1977).

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191. D. A. Micha, D. Kilin, and A. Leathers "Electronic charge transfer at a surface from the density matrix: Adsorbed metal clusters", J. Chem. Phys., to be published (2007)

Edited books

1. Proceedings of the International Symposium in Honor of John H. Van Vleck, Intern. J. Quantum Chem. Symp. **5** (J. Wiley, New York, 1971), Assistant Editor. 792 pages

2. Proceedings of the International Symposium in Honor of Sir David R. Bates, Intern. J. Quantum Chem. Symp. **17** (J. Wiley, New York, 1983), Special Editor. 650 pages

3. "Few-Body Systems and Multiparticle Dynamics" Proceedings, APS Conference, Crystal City, VA, 1987(American Institute of Physics, New York, 1987), Editor. 330 pages.

4. "Long-Range Casimir Forces: Theory and Recent Experiments in Atomic Systems" co-editors F. S. Levin and D. A. Micha (Plenum Publ. Co. , New York, 1993) . 357 pages.

5. "Coulomb Forces in Atomic and Nuclear Three-Particle Collision Phenomena" co-editors F. S. Levin and D. A. Micha (Plenum Publ. Co. , New York, 1996). 347 pages.

6. "Quantum Dynamics of Complex Molecular Systems", co-editors D. A. Micha and I. Burghardt (Springer, Heidelberg, 2007)

Scientific Reports and Manuscripts in Preparation for Publication

Scientific Reports

1. John C. Bellum and D. A. Micha "A Survey in the Fundamentals of Photon-Molecule Interactions", Univ. of Florida QTP Report, October 1981.

2. D. A. Micha and P. K. Swaminathan "Photodissociation of Polyatomics by Visible and UV Radiation: The Selfconsistent Eikonal Approximation", Univ. of Florida QTP Report TF 766R (1986).

3. Z. Parra and D. A. Micha, "Scattering of He by CO Adsorbed on Ni(001): Angular Distributions for Top- and Bridge-Sites", Univ. of Florida QTP Rep. TF 1132 (1990).

4. Z. Parra and D. A. Micha, "Energy Transfer in He Scattering by CO Adsorbed on Ni(001)", Univ. of Florida QTP Rep. TF 1139 (1990).

5. D. A. Micha "Properties of Long-Lived States in Molecular Dissociation and Scattering Phenomena" Univ. of Florida QTP Rep. 1226 (1991).

6. D. A. Micha "Theory of Collisions into Decaying Atomic States" Univ. of Florida QTP Rep. 1227 (1991).

7. E. Q. Feng and D. A. Micha "Atomic Ion-Solid Surface Collisions I. A Time-Dependent Molecular Orbital Approach", Univ. of Florida Report, September 1991.

8. E. Q. Feng and D. A. Micha "Atomic Ion-Solid Surface Collisions II. Electron Transfer in slow Na^+ - W(011) Collisions", Univ. of Florida Report, 1992.

9. S. D. Bosanac and D. A. Micha "A Model of Vibronic Transitions in Metal Atom Clusters", preprint , 1993.

Manuscripts in Preparation for Publication

1. D. Rojas and D. A. Micha "Dissipation of Energy Transferred by Collisions of Atoms into Adsorbates", in preparation for publication in Chem. Phys. Letters.

2. F. M. Fernandez and D. A. Micha "Dynamics of Dissipation in Extended Molecular Systems: an Algebraic Approach", in preparation for publication in J. Chem. Physics.

3. C. P. de Melo, B. Kirtman, and D. A. Micha "Local Space Approximation for the Time-Dependent Hartree-Fock Treatment of Electron Transfer in the Collision of Ions with Extended Systems", in preparation for publication in J. Chem. Physics.

4. D. A. Micha, "First Principles Molecular Dynamics in an Electromagnetic Field: a Density Matrix Approach", in preparation for publication in J. Chem. Physics.

5. B. Thorndyke and D. A. Micha "Quantum-classical density matrix treatment of electronically excited molecular systems: models of electron transfer and of photodissociation" in preparation for publication in J. Chem. Phys.

Papers Presented, Seminars, Colloquia, Lectures

(From September 1969)

1. Seminar, "Theoretical Aspects of Low Energy Molecular Collisions," Department of Physics, University of Florida, October 1969.

2. Paper, "Optical Potential Calculation of Molecular Vibration Excitation Cross Sections" (with M. Rotenberg), American Physical Society Meeting, Gainesville, Florida, November 1969.

3. Lectures on "Quantum Theory of Elementary Systems," Winter Institute on Quantum Theory, Part I, University of Florida, Gainesville, December 1969.

4. Lectures on "Collision Theory," Winter Institute on Quantum Theory, Part II, Sanibel Island Florida, January 1970.

5. Paper, "Many-Body Contributions to Atomic Correlation Energies," International Symposium on Quantum Theory, Sanibel Island, Florida, January 1970.

6. Seminar, "Theoretical Aspects of Low Energy Molecular Collisions," Department of Physics, Florida State University, Tallahassee, February 1970.

7. Paper, "Three-Body Description of Atom-Diatomic Molecule Reactions," American Physical Society Meeting, Dallas, Texas March 1970.

8. Seminar, "Theoretical Aspects of Low Energy Molecular Collisions," Research Institute for Engineering Sciences, Wayne State University, Detroit, Michigan, April 1970.

9. Seminar, "Vibrational Excitation of Diatomic Molecules by Atoms," Theoretical Chemistry Institute, University of Wisconsin, Madison, June 1970.

10. Lectures on "Fundamentals of Collision Theory," Summer Institute on Quantum Theory, Beistostolen, Norway, August 1970.

11. Seminar, "Theoretical Aspects of Molecular Collision Dynamics," Institute of Physical Chemistry, University of Gothenburg, Sweden, September 1970.

12. Seminar, "Molecular Compound States and Optical Potentials from the Effective Hamiltonian Method," Max-Planck-Institut fur Strömungsforschung, G—ttingen, West Germany, November 1970.

13. Lectures on "Introduction to Scattering Theory," Winter Institute on Quantum Theory, Part I, University of Florida, Gainesville, December 1970.

14. Seminar, "Collision Dynamics of Three Interacting Monovalent Atoms," Symposium on the Theory of Chemical Reactions, Rice University, Houston, Texas, April 1971.

15. Two Papers, "Many-Body Green Function Methods for Electronic Structure" and "The Three-Atom Problem in the Faddeev Formalism," Theoretical Chemistry Conference, Florida State University, Tallahassee, June 1971.

16. Paper, "Angular Distribution for the Vibrational Excitation of Diatomic Molecules by Atoms: Results for H_2 + He in the eV Region," Energy Transfer Conference, Cambridge, Great Britain, July 1971.

17. Three Papers, "Collision Dynamics of Three Interacting Monovalent Atoms," "Angular Distribution for the Vibrational Excitation of Diatomic Molecules by Atoms: Results for H_2 + He in the eV Region," and "Two-State Semiclassical Model for Penning and Associative Ionization: Collisions of $Ne(^3{}_{P2})$ with Ar, Kr and Xe," VII International Conference on the Physics of Electronics and Atomic Collisions, Amsterdam, The Netherlands, July 1971.

18. Invited Seminar, "Collision Dynamics of Three Interacting Monovalent Atoms," IV Canadian Symposium on Theoretical Chemistry, Vancouver, Canada, August 1971.

19. Seminar, "Ecuaciones de Faddeev para Sistemas de Tres Atomos," Department of Physics, University of Buenos Aires, Argentina, September 1971.

20. Paper, "Dynamical Coupling Potential in Simple Exchange Collisions: Calculations for H + H_2, D + H_2 and H + D_2," 24th Gaseous Electronics Conference, American Physical Society, Gainesville, Florida, October 1971.

21. Seminar, "Molecular Collision Dynamics: Its Program and Some of the Problems," Department of Chemistry, University of Florida, Gainesville, November 1971.

22. Two Papers, "Collision Dynamics of Three Interacting Monovalent Atoms" and "Coupled-Channel Investigation of Rotationally and Vibrationally Inelastic Collisions between He and H2," International Symposium on Quantum Theory, Sanibel Island, Florida, January 1972.

23. Seminar, "The Three-Atom Problem: Applications to Hot-Atom Reactions of Tritium with H_2," Department of Physics, University of Florida, Gainesville, April 1972.

24. Paper, "Dynamics of Hot-Atom-Diatom Collisions," Boulder Conference on Quantum Chemistry, Boulder, Colorado, June 1972.

25. Paper, "Foundation of the Spectator Stripping Model," Boulder Conference on Molecular Dynamics, Wolfeboro, New Hampshire, July 1972.

26. Seminar, "Long-Lived States in Atom-Molecule Collisions," Harvard College Observatory, Cambridge, Massachusetts, October 1972.

27. Seminar, "Role of Compound-State Resonances in Atom-Molecule Collisions," Department of Chemistry, Brandeis University, Waltham, Massachusetts, October 1972.

28. Seminar, "Faddeev Equations for a Three-Atom System," Department of chemistry, Harvard University, Cambridge, Massachusetts, October 1972.

29. Seminar, "Chemi-Ionization in Collisions with Metastable Noble-Gas Atoms," Harvard College Observatory, Cambridge, Massachusetts, November 1972.

30. Seminar, "Long-Lived States in Atom-Molecule Collisions," Department of Chemistry, Massachusetts Institute of Technology, Cambridge, November 1972.

31. Seminar, "Introduction to the Faddeev Equations," Quantum Theory Workshop, Sanibel Island, Florida, January 1973.

32. Paper, "Permutational Exchange Symmetry in Collisions Involving Identical Atoms," American Physical Society March Meeting, San Diego, California, March 1973.

33. Paper, "Single-Electron and Total Energies for Pairs of Noble Gas Atoms," American Physical Society March Meeting, San Diego, California, March 1973.

34. Seminar, "Long-Lived States in Atom Molecule Collisions," Department of Chemistry, California Institute of Technology, Pasadena, March 1973.

35. Invited Seminar, "Recent Developments in the Theory of Reactive Molecular collisions," International Symposium on Quantum Theory, Sanibel Island, Florida, January 1974.

36. Two Papers, "Interaction Potentials and Dynamics for Li + F Collisions" and "Single-Electron and Total Energies for Some Pairs of Noble Gas Atoms," International Symposium on Quantum Theory, Sanibel Island, Florida, January 1974.

37. Invited Seminar, "Recent Developments in the Theory of Molecular Collisions," Southeast Theoretical Chemistry Association, Tuscaloosa, Alabama, June 1974.

38. Communication, "Stripping Reaction of $Ar^+ + H_2$ and of $K + I_2$," Conference on Molecular Collisions, Santa Cruz, California, August 1974.

39. Lecture Series, Lectures on Quantum Theory of Molecular Collisions," I Latin American School of Theoretical Chemistry, Mexico City, Mexico, August 1974.

40. Invited Seminar, "State of Theoretical Chemistry in Latin America: Molecular Collisions Dynamics" (in Spanish), V International Conference on Theoretical Chemistry Latin Expression, Morelia, Mexico, September 1974.

41. Paper, "Dynamics of Atom-Diatomic Collisions: Isotope Effects in Ar^+ + HD Reactions" (in Spanish), V International Conference on Theoretical Chemistry Latin Expression, Morelia, Mexico, September 1974.

42. Invited Paper, "Multiple-Scattering Expansion for Molecular Collisions," V International Symposium on Quantum Theory, Sanibel Island, Florida, January 1975.

43. Paper, "Application of the Faddeev-Watson Multiple Expansion Series to Atom- Diatomic Collisions" (with J.-M. Yuan), V International Symposium on Quantum Theory, Sanibel Island, Florida, January 1975.

44. Paper, "Stripping Reactions of Alkali Atoms with Halide Diatomics" (with J. -M. Yuan), VI Southeastern Theoretical Chemistry Association, Tallahassee, Florida, June 1975.

45. Seminar, "Multiple-Collision Approach to Atom-Diatomic Scattering: Stripping Reactions in the eV Region," F.O.M. Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands, June 1975.

46. Paper, "A Many-Body Approach to Energy Transfer in Collisions of 1 - 10 eV Ions with Polyatomic Molecules," American Conference on Theoretical Chemistry, Boulder, Colorado, June 26, 1978.

47. Two Papers, "Role of Atomic-Pair Correlation Functions in Collisional Energy Transfer between Atoms and Polyatomic Molecules" and "Calculation of Energy Transfer Cross Sections for Li^+ + N_2 and Li^+ + CO Collisions: Time-of-Flight Spectra at E_{rel} = 1 - 10 eV" (with E. Vilallonga), American Chemical Society National Meeting, Miami, Florida, September 14, 1978.

48. Invited Colloquium, "State-to-State Chemistry: Impact of the Physical Method," Physics Division, Fermi National Laboratory, Batavia, Illinois, October 18, 1978.

49. Invited Colloquium, "Atom-Molecule Collisions: A Many-Body Approach," Department of Physics, Florida State University, Tallahassee, January 25, 1979.

50. Two Papers, "Rotational-Vibrational Energy Transfer in Atomic-Polyatomic Collisions: Li^+ - CO_2 and Li^+ - N_2O" (with E. Vilallonga) and "Multi-Channel Treatment of Penning Ionization in He* - Ar Collisions with Discretization of the Electronic Continuum" (with L. Relyea), International

Symposium on the Quantum Theory of Matter, Palm Coast, Florida, March 12-17, 1979.

51. Colloquium, "Scattering of Atoms by Molecules and Solid Surfaces," Department of Physics, University of Florida, Gainesville, April 26, 1979.

52. Seminar, "Role of Pair Correlation Functions in Molecular Collisions," Max- Planck Institut fur Stroemungsforschung, G—ttingen, West Germany, June 14, 1979.

53. Seminar, "Energy Transfer in Atom-Molecular Collisions: A Many-Body Approach," Department of Physics, Kaiserslautern University, West Germany, June 26, 1979.

54. Poster Session, "A Many-Body Approach to Hyperthermal Collisions: I. Energy Transfer and Dissociation in Atom-Diatom Collisions; II. Energy Transfer in Scattering by Polyatomics and Solid Surfaces," Gordon Research Conference, Wolfeboro, New Hampshire, August 16, 1979.

55. Paper, "Many-Body Perturbation Theory of Pair Correlation Functions" (with E. Vilallonga), X Southeast Theoretical Chemistry Association Conference, Tallahassee, Florida, August 25, 1979.

56. Paper, "Feshbach Formalism of Ionizing Collisions" (with L. Relyea), X Southeast Theoretical Chemistry Association Conference, Tallahassee, Florida, August 25, 1979.

57. Physical Chemistry Seminar, "Energy Transfer in Collisions of Atoms with Molecules and Solid Surfaces," University of Florida, Gainesville, October 16, 1979.

58. Colloquium, "Scattering of Atoms by Molecules and Solid Surfaces: A Many-Body Approach," Department of Physics, Georgia Institute of Technology, Atlanta, November 7, 1979.

59. Colloquium, "Energy Transfer and Reaction in Collisions of Atoms with Molecules and Solid Surfaces," Department of Chemistry, Brown University, Providence, Rhode Island, November 13, 1979.

60. Lectrue Series, "Atoms, Molecules and Atomic Collisions," Department of Physics, University of Rosario, Argentina, December 17-20, 1979.

61. Colloquium, "Energy Transfer and Reaction in Collisions of Atoms with Molecules and Solid Surfaces," Institute of Theoretical and Applied Physical Chemistry, University of La Plata, Argentina, December 27, 1979.

62. Lecture, "Hyperthermal Collisions of Atoms with Molecules and Solid Surfaces," III Workshop on Atomic Collisions, Institute of Physics, Bariloche, Argentina, January 10, 1980.

63. Four Papers, "A Correlation Function Approach to Vibrational-Rotational Energy Transfer in Atomic-Polyatomic Collisions" (with E. Vilallonga), "Electronic State Bases at Molecular Potential Pseudocrossings" (with J. Olson), "Effective Hamiltonian Theory of Ionizing Collisions" (with L. Relyea), and "Three-Body Theory of Reactive Atom-Diatom Collisions" (with Z. Kuruoglu), International Symposium on the Quantum Theory of Matter, Palm Coast, Florida, March 9-15, 1980.

64. Invited Talk, "Recent Developments in the Quantum Theory of Reactive Molecular Collisions," II West Coast Theoretical Chemistry Conference, California Institute of Technology, Pasadena, April 10, 1980.

65. Invited Review, "Few-Body Processes in Atom-Diatom Collisions," IX International Conference on the Few-Body Problem, Eugene, Oregon, August 23, 1980.

66. Invited Review, "Overview of Non-Reactive Scattering," II Chemical Congress of the North American Continent, Las Vegas, Nevada, August 29, 1980.

67. Paper, "Scattering of Ions by Polyatomics and Solid Surfaces: Multicenter Short-Range Interactions," II Chemical Congress of the North American Continent, Las Vegas, Nevada, August 29, 1980.

68. Colloquium, "Collisional Energy Transfer in Molecular Systems: A Many-Body Approach," Department of Physics, University of South Florida, Tampa, February 29, 1981.

69. Two Papers, "Cumulant Expansion of Time-Correlation Functions for Collisional Energy Transfer" and "Time-Correlation Function Approach to Anharmonic Effects in Atom-Molecule Collisions" (with E. Vilallonga), International Symposium on the Quantum Theory of Matter, Palm Coast, Florida, March 9-14, 1981.

70. Invited Paper, "Collisional Energy Transfer into Polyatomics and Solid Surfaces," American Chemical Society Florida Meeting, Tallahassee, May 7-8, 1981.

71. Invited Introductory Speaker, "Vibrational and Rotational Energy Transfer in Gases," 1981 Gordon Research Conference on Molecular Energy Transfer, Wolfeboro, New Hampshire, June 29-July 3, 1981.

72. Paper, "Cumulant Expansion of Time-Correlation Functions for Molecular Energy Transfer," 1981 Gordon Research Conference on Molecular Energy Transfer, Wolfeboro, New Hampshire, June 29-July 3, 1981.

73. Invited Speaker, "Theoretical Studies of Potential Laser Systems," NASA Workshop, Hampton, Virginia, July 13, 1981.

74. Two Papers, "Energy Transfer in Hyperthermal Collisions of Li^+ with CO_2: Effects of Molecular Anharmonicity" (with E. Vilallonga) and "Multichannel Treatment of Ionization with Discretization of the Electronic Continuum" (with R. Piacentini), XII International Conference on Physic Electronics and Atomic Collisions, Gatlinbury, Tennessee, July 15-21, 1981.

75. Seminar, "Collisional Energy Transfer into Many-Atom Systems," Oak Ridge National Laboratory, Tennessee, July 23, 1981.

76. Poster, "Collisional Excitations of Surface Phonons: A Model for Li^+ - W(110)," Gordon Conference on Dynamics of Gas-Surface Interactions, Wolfeboro, New Hampshire, August 10-14, 1981.

77. Series of Six Lectures, "Intermolecular Forces," Latin American Advanced School on Theoretical Chemistry, La Plata, Argentina, September 28-October 2, 1981.

78. Colloquium, "Energy Transfer in Molecular Collisions," Department of Chemistry, University of Montevideo, Uruguay, October 5, 1981.

79. Seminar, "Collisional Energy Transfer into Many-Body Systems: Interplay of Theory and Experiment," Department of Physics, University of Florida, Gainesville, May 18, 1981.

80. Three Papers, "A Semiclassical Treatment of Molecular Dissociation by Visible Radiation" (with P.K. Swaminathan), "An Eikonal Treatment of Non-Adiabatic Molecular Reactions" (with J. Olson), and "A Semiclassical Time-Correlation Function Approach to Inelastic Molecular Collisions: Li^+ - CO_2 and Li^+ - N_2O" (with E. Vilallonga), International Symposium on the Quantum Theory of Matter, Palm Coast, Florida, March 7-13, 1982.

81. Invited Symposium Talk, "Energy and Angular Distributions in Inelastic Atom- Polyatomic Collisions," American Chemical Society National Meeting, Las Vegas, Nevada, March 25, 1982.

82. Poster, "A Semiclassical Time-Correlation Function Approach to Atom-Polyatomic Collisions: Li^+ - CO_2 and Li^+ - N_2O in the 1 to 10 eV Range" (with E. Vilallonga), American Chemical Society National Meeting, Las Vegas, Nevada, March 24, 1982.

83. Joint Colloquium, "Scattering of Atoms by Molecules and Solid Surfaces: A Many- Body Approach," Departments of Physics and Chemistry, Drexel University, Philadelphia, Pennsylvania, May 20, 1982.

84. Invited Talk, "A Semiclassical Time-Correlation Function Approach to Collisional Energy Transfer into Many-Atom Systems," IV International Congress of Quantum Chemistry, Uppsala, Sweden, June 13-20, 1982.

85. Colloquium, "Scattering of Atoms by Many-Atom Systems," Institute of Theoretical Physics, University of California, Santa Barbara, September 15, 1982.

86. Colloquium, "Theory of Molecular Photodissociation," Department of Chemistry, University of California, Santa Barbara, October 29, 1982.

87. Lecture Series, "Molecular Scattering Theory," II Latin American Advanced School on Theoretical Chemistry, University of Montevideo, Uruguay, October 18-22, 1982.

88. Physical Chemistry Seminar, "Photodissociation of Molecules by Visible and UV Radiation," Department of Chemistry, University of Florida, Gainesville, November 16, 1982.

89. Paper, "A Semiclassical Time-Correlation Function Approach to Collisions of Li^+ Ions with CO_2 and N_2O" (with E. Vilallonga), American Physical Society Meeting, New York, January 24-27, 1983.

90. Three Papers, "Variational Determination of Self-Consistent Interactions in Atomic Collisions," "Molecular Photodissociation by Visible and UV Radiation: Time-Evolution and State-to-State Cross Sections" (with P.K. Swaminathan), and

91. "Asymptotic Expansions of Time-Correlation Functions for Energy Transfer in Molecular Collisions" (with E. Vilallonga), Bates International Symposium, Palm Coast, Florida, March 3-5, 1983.

92. Poster, "Self-Consistent Eikonal Treatment of Molecular Photodissociation and Diabatic Rearrangement" (with J. Olson and P.K. Swaminathan), American Physical Society March Meeting, Los Angeles, California, March 21-25, 1983.

93. Colloquium, "Collisional Energy Transfer into Many-Atom Systems," Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, April 12, 1983.

94. Seminar, "Variational Theory of Self-Consistent Interactions in Atomic Collisions," Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, April 14, 1983.

95. Seminar, "Collisional Energy Transfer into Many-Atom Systems," Institute of Modern Optics and Department of Physics, University of New Mexico, Albuquerque, April 22, 1983.

96. Paper, "Extension of the Time-Dependent Hartree-Fock Method to Atomic Collisions," American Physical Society Meeting, DEAP, Boulder, Colorado, June 24, 1983.

97. Paper, "Molecular Photodissociation by Visible and UV Radiation: State-to-State Cross Sections from Eikonal Distorted Waves" (with P.K. Swaminathan), XIV Southeast Theoretical Chemistry Conference, Tallahassee, Florida, June 21, 1983.

98. Seminar, "Collisional Energy Transfer Into Polyatomic Systems: A Many-Body Approach," Los Alamos National Laboratory, New Mexico, June 8, 1983.

99. Seminar, "Collisional Energy Transfer into Polyatomic Targets: A Many-Body Approach," The Hebrew University, Jerusalem, Israel, July 15, 1983.

100. Joint Physical Chemistry Seminar, "Collisional Energy Transfer into Polyatomic Targets: A Many-Body Approach," Weizmann Institute of Science, Rehovot, Israel, September 11, 1983.

101. Seminar, "Molecular Dynamics in the Presence of Electronic Rearrangement," Chemistry Department, University of Florida, November 15, 1983.

102. Seminar, "An Extended Time Dependent Hartree-Fock Method for Molecular Interactions," Quantum Theory Project, University of Florida, February 27, 1984.

103. Three Papers, "State-to-State Cross Sections for Photodissociation of Polyatomic Molecules by Visible and UV Radiation," (with P.K. Swaminathan); "Excitation of Harmonic Molecular Modes by Non-Linear Forces," (with B. Gazdy); and "Distribution of Final Energies in Collisions of Li^+ and N_2: A Semiclassical Time-Correlation Function Treatment," (with E. Vilallonga), International Symposium, Palm Coast, March 5-10, 1984.

104. Invited Symposium Paper, "Model Calculations of H + H_2 Resonances within a Many- Body Approach to Reactive Scattering," National ACS Meeting, St. Louis, April 8-13, 1984.

105. Chemical Physics Seminar, "Collisional Energy Transfer into Polyatomic Targets: A Many-Body Approach," Oak Ridge National Laboratory, Tennessee, June 25, 1984.

106. Invited Talk, "Scattering by Polyatomic Targets: A Time-Correlation Function Approach," Gordon Conference, Wolfeboro, New Hampshire, August 13-17, 1984.

107. Seminar, "Time-Correlation Functions for Molecular Collisions Using Path Integrals," Quantum Theory Project, University of Florida, February 13, 1985.

108. Invited talk, "Collisional Time-correlation Functions for Molecular Interactions," Sanibel Symposia, Marineland, Florida, March 14-23, 1985.

109. Four Papers, 1) "Exact Time-correlation Function for the Linearly Driven Parametic Oscillator" (with B. Gazdy); 2) "Energy Transfer in the Collision of Parametic Oscillator" (with J. Recamier and B. Gazdy); 3) "Vibrational Modes and Collisional Excitation of CO Adsorbed on Ni(001)" (with Z. Parra); 4) "Quantum Yields for Photodissociation of Polyatomic Molecules by Visible and U.V. Radiation" (with C. Stodden), Sanibel Symposia, Marineland, Florida, March 14-23, 1985.

110. Paper, "Photodetachment of Atomic Electrons in Magnetic Fields" (with O. Crawford), 16th Annual Meeting Div. El. and At. Phys., APS, Norman Oklahoma, May 29-31, 1985.

111. Invited Talk, "Collisional Energy Transfer into Polyatomic Molecules," Gordon Conference, Wolfeboro, New Hampshire, July 8-12, 1985.

112. Award Talk, "Matter in Transition: The Molecular Viewpoint," Society of Sigma Xi and Division of Physical Chemistry, Univ. of Florida, October 8, 1985.

113. Seminar, "Collisional Energy Transfer into Polyatomic Systems," Chemistry Department, Florida State University, November 4, 1985.

114. Paper, "Variational Improvement of the Time-Dependent Hartree-Fock Method: Application to He + He^{2+} and He^{+} + He^{+} Collisions" (with B. Gazdy), Sanibel Symposia, Marineland, Florida, March 6-15, 1986.

115. Invited talk, "Extensions of the Time-Dependent Hartree-Fock Method and Applications to Atomic Collisions," Snowbird (Utah) Conference, April 21-26, 1986.

116. Paper, "Variational Improvement of the Time-Dependent Hartree-Fock Method for Atomic Collisions," APS National Meeting, Washington DC, April 28-May 1, 1986.

117. Invited talk, "Transition Probabilities for Atomic Collisions using a Variational Many-Electron Theory," SETCA Meeting, Tallahassee, May 22-24, 1986.

118. Seminar, "Energy Transfer into Complex Polyatomic Targets Using Collisional Time-Correlation Functions," Naval Research Laboratory, Washington, D.C., May 2, 1986.

119. Four Papers, 1) "Vibrational Excitation in Collisions between Two Diatomic Molecules Using an Operator Algebra"(with B. Gazdy); 2) "Energy Transfer in Impulsive Collisions of Light Atoms with CO Adsorbed on Ni(001)" (with Z. Parra); 3) "Time-Correlation Function Approach to the Interaction of Light with Polyatomic Systems" (with D. Srivastava); 4) "Self-Consistent Eikonal Treatment of Polyatomic Photodissociation" (with C. Stodden), SETCA Meeting, Tallahassee, May 22-24, 1986.

120. Invited talk, "Energy Transfer into Polyatomic Targets: A Collisional Time- Correlation Function Approach," Conference Collision Dynamics of Clusters and Long-lived States, Brioni (Yugoslavia), Sept. 1-5, 1986.

121. Seminar, "Transition Probabilities for Atomic Collisions Using a Variational Many-Electron Theory," Institute for Atomic Physics, Stockholm, Sweden, Aug. 1, 1986.

122. Seminar, "Transition Probabilities for Atomic Collisions Using a Variational Many-Electron Theory," Department of Quantum Chemistry, Uppsala University, Aug. 11, 1986.

123. Four papers, 1) "Energy Transfer in Scattering of Atoms by Molecules Adsorbed on Metal Surfaces" (with Z. Parra); 2) "Molecular State-to-State Transition Probabilities from Eikonal Wave Functions" (with C. Stodden); 3) "Collisional Time Correlation Function Approach to the Interaction of Light with a Polyatomic System" (with D. Srivastava); 4) "Charge Transfer in Ion-Surface Collisions: A Time Dependent Self Consistent Field Approach" (with Q. Feng), Sanibel International Symposia, Marineland, Florida, March 16-21, 1987.

124. Invited talk, "Transferencia de energia en colisiones moleculares usando funciones de correlacion temporales" V Congreso Argentino de Fisicoquimica, Mar del Plata, Argentina, April 28, 1987. (Plenary Lecture).

125. Two seminars, "Transferencia de energia en colisiones moleculares"; "Funciones de correlacion para colisiones moleculares en el limite semiclasico," Physics Department, Univ. Nacional de Buenos Aires, May 5, 1987 and May 15, 1987.

126. Seminar, "Quimica Teorica en la Universidad de Florida," Chemistry Department, Universidad Nacional de Buenos Aires, Argentina, May 14, 1987.

127. Two contributed papers, "The Effect of Intra- and Intermolecular Media on the Interaction of Light with a Polyatomic System" (with D. Srivastava); "Charge Transfer in Ion-Surface Collisions: A Time-Dependent Self-Consistent Field Approach" (with Q. Feng), XVI SETCA Meeting, Florida State University, Tallahassee, FL., May 21-23, 1987.

128. Invited talk, "Time-Dependent Hartree-Fock and its Extensions for Atomic Interactions," Ruder Boskovic Institute, Zagreb, Yugoslavia, June 17, 1987.

129. Invited talk, "Time-Dependent Variational Functionals for Atomic Interactions", MATH/CHEM/COMP 1987 Conference, Dubrovnik, Yugoslavia, June 22-26, 1987.

130. Invited symposium talk, "Translational-to-Rovibrational Energy Transfer at Hyperthermal Velocities: Approaches Based on Collisional Time-Correlation Functions", Conference on the Dynamics of Molecular Collisions, Wheeling, West Virginia, July 12-17, 1987.

131. Chemistry colloquium, "Quantum Molecular Dynamics and Some of its Applications", University of Nevada, Reno, December 18, 1987.

132. Four contributed papers, "Application of the Self-Consistent Eikonal Approximation to Branching Ratio Calculations of the Photodissociation of CH_3I," (with C. Stodden); "Angular Distribution of Atoms Inelastically Scattered by Adsorbed Molecules" (with Z. Parra); "Localized Time-Dependent Molecular Orbitals for Charge Transfer in Ion-Surface Collisions" (with Q. Feng); "Path- Integral Formulation of Molecular Light Absorption Using a Time-Dependent SCF Approximation" (with D. Srivastava), Sanibel International Symposia, Marineland, Florida, March 12-19, 1988.

133. Contributed paper, "Time-Correlation Function Approach to Photodissociation in Extended Molecular Systems" (with D. Srivastava), American Physical Society National Meeting, New Orleans, March 21-25, 1988.

134. Physical Chemistry Seminar, "Interaccion de la Radiacion Con Sistemas Moleculares Extensos," Chemistry Department, Universidad de Buenos Aires, May 19, 1988

135. Two contributed posters (1) "Energy and Angular Distributions of Atoms Scattered by Adsorbates," (with Z. Parra); (2) "Photodissociation in Extended Molecular Systems," (with D. Srivastava), Gordon Conference on "Atomic and Molecular Interactions," Aug. 1-5, 1988, Plymouth, New Hamshire.

136. Seminar, "Dinamica Molecular Cuantica de la Photodisociacion," INIFTA, Chemistry Department, Universidad Nacional de La Plata, Argentina, Oct. 11, 1988.

137. Seminar, "Ways and Means of Quantum Molecular Dynamics," Chemistry Department , University of Florida, Physical Chemistry, Fall 1988.

138. Colloquium, "Dynamics of Polyatomics and Adsorbates: Photodissociation and Collisional Energy Transfer," Chemistry Department, Emory University, Feb. 28, 1989.

139. Four contributed papers: 1) "Time-dependent SCF Theory of Molecular Interactions" (with K. Runge); 2) "Electron Transfer in Atom-Surface Interactions in a Basis of Localized Electronic States" (with Q. Feng); 3) "Photodissociation of Vibrationally Excited CH_3I in a TDSCF Approximation" (with D. Srivastava); 4) "Three-Body Calculations of the $H+H_2$ Reaction" (with Zeki C. Kuruoglu) Sanibel International Symposia, St. Augustine, Florida, April 1-8, 1989.

140. Invited lecture, "Photodissociation and the Interaction of Adsorbed Atoms with Metal Clusters," R. Boskovic Institute, Zagreb, Yugoslavia, June 22, 1989.

141. Invited talk, "Calculation of Time Correlation Functions in Quantum Molecular Dynamics," MATH/CHEM/COMP Conference, Dubrovnik, Yugoslavia, June 26-July 1st 1989.

142. Contributed paper, "Electronic Rearrangement in Molecular Collisions: A TDMO Approach" (with K. Runge and Q. Feng), Conf. Dynamics of Molecular Collisions, Asilomar, California, July 16-21, 1989.

143. Contributed paper, "Photodissociation Dynamics of Extended Polyatomic Systems" (with D. Srivastava), Amer. Chem. Soc. National Meeting, Miami Beach, Florida, Sept. 10-15, 1989.

144. Invited talk, "Dinamica de Disociacion en Sistemas Moleculares Extensos," XVIII Congreso Internacional de Quimicos Teoricos de Expresion Latina, La Plata, Argentina, Sept. 23-28, 1989.

145. Colloquium, "Photodissociation Dynamics in Extended Molecular Systems" Physics Department, University of Puerto Rico, Feb 22, 1990.

146. Invited Short Paper and Poster "Many-Electron Treatment of Electron Transfer and Polarization in Atomic Interactions" (D. A. M., K. Runge and Q. Feng), Amer. Phys. Soc. National Meeting, Anaheim, CA, March 12-16, 1990.

147. Five contributed papers: 1) "Minimal Potential Energy Structures of Co^+Ar_n and V^+Ar_n Cluster Ions Via Similated Annealing" (R. L. Asher, DAM, and P. J. Brucat); 2) "Orientation of Atomic Orbitals in Ion-Solid Surface Collisions: a Time-Dependent MO Approach" (Qun Feng and DAM); 3) "Coupling of Electronic and Nuclear Motions in Atomic Collisions Using a Time-Dependent MO Approach" (K. Runge and DAM); 4) "The Effect of Oscillator Strengths on the Angular Distributions and Branching Ratios of Photodissociation Products" (C. D. Stodden and DAM); 5) "The Eikonal Approximation Applied to Electronically Diabatic Molecular Interactions" (J. Cohen and DAM), Sanibel International Symposia, St. Augustine, Florida, March 17-24, 1990.

148. Invited talk,"Time-dependent Molecular Orbital Theory of Atomic Interactions"(DAM), XIX Southeastern Theor. Chem. Assoc. Conf., Tallahassee, Florida, May 17-19 (1990)

149. Three contributed papers, XIX Southeastern Theor. Chem. Assoc. Conf., Tallahassee, Florida, May 17-19 (1990): 1) "Minimal Potential Energy Structures of Co^+Ar_n and V^+Ar_n Cluster Ions Via Similated Annealing" (R. L. Asher, DAM, and P. J. Brucat); 2) "Coupling of Electronic and

Nuclear Motions in Atomic Collisions Using a Time-Dependent MO Approach" (K. Runge and DAM); 3) "Electron Transfer at Solid Surfaces" (E. Q. Feng and DAM)

150. Contributed paper "Classical Trajectory Calculations for Co^+Ar_n, ^+Kr_n, $V^+Ar_n$and V^+Kr_n Cluster Ions" (R. Asher, DAM and P.J. Brucat), 1990 Florida Annual Meeting, Amer. Chem. Soc., Jacksonville, Florida, May31-June2, 1990.

151. Invited Lecture Series"Interaction of Light with Extended Molecular Systems: Photodissociation" (DAM), Escuela Latinoamericana de Fisica, Caracas, Venezuela, July 23-Aug. 3, 1990.

152. Seminar "Electron Transfer in Low Energy Atomic Collisions: A Time-Dependent Molecular Orbital Approach" Harvard University, Institute for Theoretical Atomic and Molecular Physics, Oct. 29, 1990.

153. Seminar "Photodissociation in Extended Molecular Systems", Division of Physical Chemistry, Florida State University, Feb. 11, 1991.

154. Chemistry Colloquium "Electron Transfer Phenomena in Molecular Interactions", Chemistry Department, Florida State University, Feb 22, 1991.

155. Invited Talk "Time-Dependent Molecular Orbital Theory of Electron Transfer in Slow Atomic Collisions", Harvard University Workshop on Time-Dependent Phenomena, Center for Astrophysics, Cambridge, Mass, March 1-3, 1991.

156. Three contributed papers: 1) "Conformational Changes in Clusters of a Transition Metal Ion and Rare Gas Atoms from a Simulated Annealing Method" (R. L. Asher, DAM, and P. J. Brucat); 2) "Polarization Effects in Ion-Atom Collisions Using a Time-Dependent Molecular Orbital Approach" (K. Runge and DAM); 3) "A Study of Effective Potentials for Electronically Diabatic Atom-Atom Collisions" (J. Cohen and DAM), Sanibel International Symposia, St. Augustine, Florida, March 9-16, 1991.

157. Seminar "Electron Transfer Phenomena in Molecular Interactions", Chemistry Department, Phys. Chem. Division, Univ. of Florida, April 23, 1991.

158. Contributed paper "A Study of Effective Potentials for Electronically Diabatic Atom-Atom Collisions"(J. Cohen and DAM), Annual Meeting Florida Section of the ACS, Tampa, May 16-18, 1991.

159. Seminar "Computational Challenges in Quantum Molecular Dynamics", Supercomputer Computational Research Institute, Florida State University, May 22, 1991.

160. Chemistry Colloquium "Electron Transfer Phenomena in Molecular Interactions", Embry-Riddle Aeronautical University, Daytona Beach, September 10, 1991.

161. Seminar " A Time-Dependent Molecular Orbital Approach to Slow Atomic Collisions", Inst. for Theoretical Physics, Univ. of California, Santa Barbara, October 22, 1991.

162. Four contributed papers, Sanibel International Symposia, St. Augustine, Florida, March 14-21, 1992:

    (a) "Time-Correlation Functions and Rate Coefficients for Transition Metal Ion-Rare Gas Clusters Using Classical Dynamics" (R. L. Asher, DAM, and P. J. Brucat)

    (b) "Time-Evolution of Electronic Populations and Polarization Parameters in Slow Ion-Atom Collisions" (K. Runge and DAM)

    (c) "Calculation of Reaction Rate Constants from Collisional Time-Correlation Functions for Diatomic and Triatomic Systems" (D. Beksic and DAM)

    (d) Electronically Diabatic Effects on the Branching Ratios of CH_3I Photodissociation"(C. D. Stodden and DAM)

163. Invited Talk "Electronic Energy and Charge Transfer in Slow Atomic Collisions: A Time-Dependent Molecular Orbital Approach", NATO Advanced Research Workshop, Snowbird, Utah, March 30-April 3, 1992.

164. Colloquium "Modelling Electron Transfer in Molecular Interactions", Beckman Institute, University of Illinois, Urbana, June 10 (1992).

165. Selected paper "Electron Transfer in Ion-Atom and Ion-Solid Metal Interactions Using a Time-Dependent Molecular Orbital Approach"(D. A. Micha and Keith Runge), National Amer. Chem., Soc. Meeting, Washington, DC, August 24-27 (1992).

166. Selected paper "Isomerization Rates for Transition Metal Ion-Rare Gas Clusters Using Simulated Annealing and Molecular Dynamics" (R. Asher, D. A. Micha and P. Brucat), National Amer. Chem., Soc. Meeting, Washington, DC, August 24-27 (1992).

167. Seminar "Electron Transfer in Condensed Media: the Marcus Theory Revisited", Physical Chemistry Div., Univ. of Florida, November 12 (1992).

168. Colloquium "Electron Transfer Phenomena in Molecular Interactions", Chemistry Department, Univ. of Miami, Feb. 3, 1993.

169. Lectures "Quantum Molecular Dynamics", US-Latin American Workshop on Molecular and Materials Sciences: Theoretical and Computational Aspects, UF, March 10-12, 1993.

170. Four contributed papers, Sanibel International Symposia, St. Augustine, Florida, March 13-20, 1993:

    (a) "Isomerization Rates of Clusters from Constrained Molecular Dynamics" (R. L. Asher, DAM, and P. J. Brucat)

(b) " Time-Correlation Functions for Electronically Diabatic Phenomena Using the Lanczos Reduction Method" (D. Beksic and DAM)

(c) "Time-Dependent Atomic Orbital Basis Sets for Molecular Interactions" (H. da Costa and DAM)

(d) "Time-Evolution of Two Active Electrons in Slow Atomic Collisions" (K. Runge and DAM)

171. Special Seminar, "Temporal Evolution of Electron Densities in Slow Atomic Collisions" Weizmann Institute, Rehovot, Israel, June 9, 1993.

172. Seminar, "Electron Transfer in Slow Atomic Collisions" Dep. de Fisica Fundamental, Consejo Superior de Investigaciones Cientificas, Madrid, Spain, June 25, 1993.

173. Invited talk "Temporal Evolution of Electron Densities in Slow Atomic Collisions" I Intern. Congress on Theor. Chem. Physics, Girona, Spain, June 28-July 3, 1993.

174. Poster, "Electronically Diabatic Dynamics of Molecular Photodissociation and Collisional Processes Using Wavepackets"(D. Beksic and DAM) I Intern. Congress on Theor. Chem. Physics, Girona, Spain, June 28-July 3, 1993.

175. Poster "Electron Transfer Probabilities in Slow Ion-Metal Surface Collisions" (DAM and E. Q. Feng) Gordon Conf. Dynamics of Gas-Surface Interactions, Andover, New Hampshire, Aug. 2-6, 1993.

176. Invited Talk "Temporal Evolution of Electronic Densities in Slow Atomic Collisions", IX Congreso Costarricense de Fisica, San Jose, Costa Rica, 8-13 November, 1993.

177. Invited Talk, "Mecanica Cuantica, Atomos y Moleculas" V Short Course for Docent Extension, Universidad Nacional, San Jose, Costa Rica, 5-13 November, 1993.

178. Lectures "Time Scales in Ab Initio Quantum Molecular Dynamics", 1994 US-Latin American Workshop on Molecular and Materials Sciences: Theoretical and Computational Aspects, UF, February 8-10, 1994.

179. Four contributed papers, Sanibel International Symposia, Sawgrass, Florida, February 12-19, 1994:

(a) "A Study of Intermediate Species in the Isomerization of Ion Clusters Using Constrained Molecular Dynamics" (R. L. Asher, DAM, and P. J. Brucat)

(b) " Photodesorption Dynamics Using Time-Correlation Functions: a Model for CO(ads)Ni(001)" (D. Beksic, DAM, and K. Runge)

(c) "Self-consistent Coupling of Atomic Orbital Exponents to a Moving Charge" (H. da Costa and DAM)

(d) "The Role of d-Orbitals in Slow Ion Collisions: Time-dependent Polarization and Charge Transfer" (K. Runge and DAM)

180. Contributed paper "A Time-Dependent Many-Electron Approach to Atomic and Molecular Interactions" (K. Runge and DAM) Amer. Phys. Soc. Meeting, Crystal City, VA, April 18-22. 1994.

181. Invited Plenary Talk "Time-dependent Many-Electron Theory of Collisional Electron Transfer"(DAM) , MOLEC X European Conference, Salamanca, Spain, Aug. 28-Sep. 2, 1994.

182. Poster "Quantum Dynamics of the Photodesorption of CO from the Ni(001) Surface" (D. Beksic and DAM) MOLEC X European Conference, Salamanca, Spain, Aug. 28-Sep. 2, 1994.

183. Chemistry Colloquium "Electron Transfer in Molecular Interactions", Baylor University, Texas, Oct. 14th, 1994.

184. Physics Seminar, "Time-Dependent Many-Electron Theory of Collisional Energy Transfer", Univ. of Nevada, Las Vegas, Oct. 28th, 1994

185. Physical Chemistry Seminar "Computational Chemistry with a PC: A Tutorial", Univ. of Florida, Nov. 1st, 1994.

186. Three contributed papers, Sanibel International Symposia, St. Augustine, Florida, Feb. 25-March 4, 1995:

(a) D. Beksic, Z-G.Yi and D. A. M. "Distribution of Final Energies of CO Photodesorbed from Ni(001): a Quantum Dynamics Study"

(b) H. F. DaCosta, D. A. M. and K. Runge "Time-evolution of Light Emitted in Slow Ion-Atom Collisions"

(c) K. Runge and D. A. Micha "Time-Evolution of Orbital Polarization in Slow Ion-Atom Collisions with Two Active Electrons"

187. Oral presentation, D. A. M. and D. Beksic "Quantum Dynamics of CO Photodesorption from the Ni(001) Surface", Amer. Phys. Soc. National Meeting, March 20-24, 1995, San Jose, California

188. Colloquium "Interaccion de Radiacion Electromagnetica con Moleculas Adsorbidas sobre Metales", Physics Department, Univ. of Buenos Aires, May 22, 1995, Argentina.

189. Invited Talk "Dependencia Temporal de Propiedades en Colisiones Atomicas", workshop Reunion sobre Estructura Electronica y Teoria de Colisiones, Univ. de Buenos Aires, May 23-24, 1995, Argentina.

190. Seminar "Quantum Dynamics of CO Photodissociation from the Ni(001) Surface", Chemistry Department, Univ. of Tennessee (Knoxville), Oct. 2, 1995.

191. Three contributed papers, Sanibel International Symposia, St. Augustine, Florida, Feb. 24-March 2, 1996:

    (a) Z.-G. Yi, D. Beksic, and D. A. M. "Time-evolution of CO Vibrational Populations in Photodesorption by Light Pulses"

    (b) H. F. M. DaCosta, D. A. M., and K. Runge "Intensity and Polarization of Light Emitted in Slow Ion-Atom Collisions"

    (c) K. Runge and D. A. Micha, "Time-evolution of Many Active Electrons in Slow Ion-Atom Collisions"

192. Selected talk, D. A. M. "Quantum Dynamics of Molecular Desorption: CO on Ni(001)", Intern. Congress Theoret. Chem. Physics, New Orleans, April 8-13, 1996

193. Contributed paper, K. Runge and D. A. M. "Time-evolution of Many Active Electrons in Slow Ion-Atom Collisions", Amer. Phys. Soc. Div. At. Mol. Opt. Phys., Ann Arbor, Michigan, May 15-18, 1996.

194. Contributed paper, H. F. M. DaCosta, D. A. M., and K. Runge "Transient Light Emitted from Slow Ion-Atom Collisions: Intensity and Polarization", Amer. Phys. Soc. Div. At. Mol. Opt. Phys., Ann Arbor, Michigan, May 15-18, 1996.

195. Seminar, D. A. M., "Time-dependent Many-electron Theory of Electronic Energy and Charge Transfer in Molecular Interactions", Max Plack Institut fuer Astrophysik, Garching, Germany, May 14, 1996

196. Colloquium, D.A.M. "Quantum Dynamics of CO Desorption from Metal Surfaces", Physics Department, Wuerzburg University, Germany, May 21, 1996.

197. Colloquium, D.A.M. "Quantum Dynamics of CO Desorption from Metal Surfaces", Inst. Theoret. and Phys. Chemistry, Freie Universitet, Berlin, Germany, June 19, 1996.

198. Seminar, D.A.M. "Quantum Dynamics of Photodesorption of Diatomics from Metal Surfaces", Max Planck Inst. fuer Stroemungsforschung, Goettingen, Germany, June 21, 1996.

199. Seminar, D.A.M. "Quantum Dynamics of Photodesorption of Diatomics from Metal Surfaces", Physics Department, Technische Universitet Munich, Germany, June 26, 1996.

200. Seminar, D. A. M., "Transient Light Emission in Slow Ion-Atom Collisions", Max Plack Institut fuer Astrophysik, Garching, Germany, June 27, 1996

201. Seminar, D.A.M. "Time-evolution of Electron Transfer and Light Emission in Ion Collisions", Max Planck Inst. fuer Stroemungsforschung, Goettingen, Germany, July 7, 1996.

202. Contributed paper, K. Runge and D. A. M. ""Time-evolution of Many Active Electrons in Slow Ion-Atom Collisions", Amer. Theoret. Chem. Conference, Park City, Utah, July 21-25, 1996.

203. Selected talk, D. A. M. and Z-G. Yi, "Quantum Dynamics of CO Photodesorption from Metal Surfaces by Visible and UV Light Pulses", National ACS Meeting, Orlando, FL, Aug. 25-29, 1996.

204. Contributed paper, K. Runge and D. A. M. "Time-evolution of Orbital Polarization Parameters in Slow Ion-Atom Collisions Involving Several Active Electrons", National ACS Meeting, Orlando, FL, Aug. 25-29, 1996.

205. Seminar, D. A. M. "Time-Dependent Many-electron Theory of Collisional Light Emission", Quantum Theory Project, Univ. of Florida, Gainesville FL, Sep.19, 1996

206. Invited talk, D. A. M. "Quantum Molecular Dynamics: from Simple to Complex Systems", Swedish-American Symposium on the Foundations of Quantum Theory in Chemistry, Molecular Physics, and Biology, Sanibel Island, Florida, Oct. 26-29, 1996.

207. Seminar, D. A. M. "Femtosecond Dynamics of Molecular Photodesorption from Metal Surfaces", Joint Condensed Matter and Chemical Physics seminar, Univ. of Florida, Gainesville FL, Nov. 4, 1996

208. Three contributed papers, Sanibel International Symposia, St. Augustine, Florida, March 1-8, 1997:

    (a) H. F. DaCosta, D. A. M. and K. Runge "Time and Frequency Dependence of Light Emitted in Slow Ion-Atom Collisions"

    (b) K. Runge and D. A. Micha "Cross Sections for Electronic Rearrangement in Slow Ion-Atom Collisions Involving Many Active Electrons"

    (c) Z-G. Yi and D. A. M. "Femtosecond Dynamics of CO Photodesorption from Metal Surfaces by Light Pulses"

209. Invited Symposium paper, D.A.M. and Z. Yi "CO Photodesorption from the Cu Metal Surface: Femtosecond Dynamics with Visible and UV Light Pulses" Amer. Chem. Soc. Florida Section, Orlando FL, May 2-3, 1997.

210. Seminar D. A. M. "Femtosecond Dynamics of Molecular Photodesorption from Metal Surfaces", J. Heyrovskeho Institute of Physical Chemistry, Prague, Czeck Republic, May 26, 1997

211. Seminar D. A. M. "Molecular Dynamics of Elerctronically Excited Systems: Electron Transfer and Light Emission", Technical University, Munich, May 28, 1997.

212. Seminar D. A. M. "Femtosecond Dynamics of Molecular Desorption from Metal Surfaces", Department of Chemistry University College, London, June 9, 1997.

213. Invited Symposium Talk, D. A. M. "Electronic Excitation and Quantum Dynamics of CO Photodesorption from Cu and Ni Metal Surfaces" V Chemical Congress of North America, Can-Cun, Mexico, Nov. 11-15, 1997.

214. Colloquium Talk, D. A. M. "Time-Evolution of Radiation Emitted in Ion-Atom Collisions", Clark-Atlanta University NSF Center for Theor. Studies of Phys. Systems, January 9, 1998.

215. Three contributed papers, Sanibel International Symposia, St. Augustine, Florida, February 21-27, 1998:

    (a) H. F. DaCosta, D. A. M. and K. Runge "Time Dependence of Spin-Orbit Coupling in Slow Ion-Atom Collisions" (presented only by title)

    (b) D. A. Micha and K. Runge "Time-Dependence of Electronic Rearrangement and State-to-State Cross Sections for Slow Collisions Involving Several Active Electrons"

    (c) Z-G. Yi and D. A. M. "Linear and Nonlinear Yields of CO Photodesorbed from a Cu Metal Surface by Light Pulses"

216. Invited Talk, D. A. M. "Femtosecond Dynamics of Photodesorption: Nonlinear Yields for CO/Cu", (Symposium on Femtosecond Dynamics at Surfaces: Theory and Experiment) Amer. Physical Soc. National Meeting, March 16-20, 1998, Los Angeles.

217. Invited Talk, D. A. M. "Femtosecond Dynamics of Photodesorption: Density Matrix Theory for CO/Cu", 27th SETCA Meeting, FSU, Tallahassee, May 27-28, 1998.

218. Two contributed papers, 27th SETCA Meeting, FSU, Tallahassee, May 27-28, 1998:

    (a) Akbar Salam and D. A. M. "Non-linear Optical Response in the Femtosecond Photodesorption of Molecules from Metal Surfaces"

    (b) Brian Thorndyke, D. A. M. and K. Runge "Time-dependent Many-electron Treatment of Electronic Rearrangement in Atomic Collisions".

219. Invited Short Talk, D. A. M., Z. Yi and A. Salam, "Femtosecond Dynamics of CO Photodesorption from Cu Metal Surfaces: Nonlinear Phenomena and Optical Control", Gordon Conference on Atomic and Molecular Interactions, New London, NH, June 28-July 3, 1998

220. Poster, B. Thorndyke, K. Runge and D. A. M., "Time-dependent Many Electron Treatment of Electronic Rearrangement in Slow Ion-Atom Collision", Gordon Conference on Atomic and Molecular Interactions, New London, NH, June 28-July 3, 1998

221. Seminar, D. A. M. "Transient Light Emission in Slow Ion-Atom Collisions", Harvard University Institute for Theoretical Atomic and Molecular Physics, July 7, 1998

222. Seminar, D. A. M. and J-M. Yuan "Time-resolved spectroscopy: pulses, chirping, and related topics", Harvard University Institute for Theoretical Atomic and Molecular Physics, July 9, 1998

223. Colloquium, D. A. M. "Quantum Molecular Dynamics: What is New" Physics Department, Univ. of Florida, Jan. 7, 1999.

224. Invited talk, D. A. M. "First Principles Quantum Molecular Dynamics of Electronic Excitation and Charge Transfer", US-Latin America-Canada-Caribbean Workshop on Molecular and Materials Sciences", Cuernavaca, Mexico, Feb. 24-26 (1999).

225. Three contributed papers, Sanibel International Symposia, St. Augustine, Florida, February 27-March 5, 1999:

    (a) B. Thorndyke, D. A. M., K. Runge, and A. Reyes "Acceleration Effects in Slow Ion-Atom Collisions from a First Principles Dynamics"

    (b) A. Salam and D. A. M. "Theory of the Nonlinear Optical Response of Metal Surfaces: the CO/Cu(001) System"

    (c) A. Santana, D. A. M., and Z-G. Yi "Temperature Effects on the Photodesorption of CO from Cu(001)"

226. Poster, B. Thorndyke, D. A. M., and K. Runge, "Electronic Energy and Charge Transfer in Slow Ion-Atom Collisions from a First Principles Dynamics: Acceleration Effects", American Physical Society Centennial Meeting, Atlanta, March 20-26, 1999.

227. Seminar, D. A. M., "Dinamica Cuantica Molecular de Fotodesorcion Inducida por Pulsos de Luz", QUINOR, Dep. of Chemistry, Univ. Nacional de La Plata, Argentina, May 7, 1999.

228. Seminar, D. A. M., "Dinamica Molecular Cuantica con un Metodo Ab Initio: Colisiones de Iones en Gases y con Superficies", Instituto de Fisica, Univ. Nacional de Cuyo, Bariloche, Argentina, May 10, 1999.

229. Seminar, D. A. M., "Dinamica Cuantica Molecular Inducida por Pulsos de Luz", Dep. of Physics, Univ. Nacional de Buenos Aires, Argentina, May 13, 1999.

230. Invited talk, D. A. M. "Electronic Energy and Charge Transfer in Slow Ion-Atom Collisions from a First Principles Quantum Dynamics: Systems with Several Active Electrons", Amer. Chem. Soc. National Meeting, New Orleans, Aug. 25, 1999

231. Two contributed papers, Univ. of Florida 1999 Research Affiliates Meeting, Poster Session.

    (a) A. Reyes, K. Runge, B. Thorndyke, and D. A. M. "Using Effective Core Potentials for Atoms in a First Principles Molecular Dynamics "

    (b) A. Santana and D. A. M. "Temperature Effects on the Photodesorption of CO/Cu(001): Yields of Final Vibrational States and Non-Boltzmann Distributions"

232. Invited talk, "Time-dependent Many-electron Treatment of Electronic Excitation and Charge Transfer in Slow Ion-Atom Collisions", Inst. Theoret. At. and Molec. Physics, Harvard University, Nov. 4-6, 1999.

233. Invited plenary talk "Density Matrix Theory and Computational Aspects of Quantum Dynamics in a Medium", III Congress Intern. Soc. Theoret. Chemical Physics, Mexico City, Nov. 8-13, 1999

234. Seminar, D. A. M., "Density Matrix Theory and Computational Aspects of Quantum Dynamics in a Medium: Photodesorption of CO/Cu(001)" Chemistry Department, Univ. of California Irvine, Jan. 7, 2000.

235. Seminar, D. A. M., "Density Matrix Theory of Quantum Dynamics in an Active Medium", Quantum Theory Project, Univ. of Florida, Feb. 16, 2000.

236. Three contributed papers, Sanibel International Symposia, St. Augustine, Florida, February 26-March 3, 2000:

    (a) A. Reyes, K. Runge, B. Thorndyke, and D. A. M. "Electronic Excitations in Atom-Atom Collisions from a First Principles Dynamics using Effective Atomic Core Potentials"

    (b) A. Santana-Vargas, A. Salam and D. A. M. "Density Matrix Calculation of Nonlinear Yields of Diatomics Photodesorbed by Femtosecond Pulses"

    (c) B. Thorndyke and D. A. M. "Density Operator Treatment of Coupled Classical-Quantal Dynamics and Time-Dependent Many-Electron Systems"

237. Chemical Physics Seminar, D. A. M. "Quantum dynamics of electronic energy and charge transfer", California Institute of Technology, Pasadena CA, April 18, 2000.

238. Seminar, D. A. M. "Femtosecond spectra and dynamics in active media: photodesorption of diatomics", ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, April 20, 2000.

239. Oral presentation, D. A. M. "Atom-atom inelastic collisions from a first principles dynamics using effective atomic core potentials", DAMOP Amer. Phys. Soc. Meeting, Storrs, CN, June 15, 2000.

240. Lecture series, D. A. M. "Quantum dynamics in an active medium: the example of femtosecond desorption", Gordon Summer School on Theoretical Chemical Physics, Bristol RI, June 22-23, 2000.

241. Poster presentation, D. A. M., A. Santana, and A. Salam " The dissipative dynamics of diatomics photodesorbed from metal surfaces by femtosecond light pulses", Gordon Research Conference on Atomic and Molecular Interactions, New London, NH, July 2-7, 2000.

242. Poster presentations, Zerner Memorial Meeting, Univ. of Florida, Gainesville, Nov. 16-18 (2000)

    (a) A. Reyes, K. Runge and D. A. M. "Alkali-RareGas atomic interactions from a first principles dynamics using effective atomic core potentials"

    (b) A. Santana and D. A. M. "Adsorbate vibrational effects on the photodesorption of CO from Cu(001)"

243. Invited talk, D. A. M. (with A. Santana and A. Salam) "Nonlinear yields of diatomics photodesorbed by femtosecond pulses: density matrix theory and calculations", Amer. Chem. Soc. Pacifichem Meeting, Honolulu, Dec. 12 (2000)

244. Invited talks, Institute for Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, Dec. 21 and 22 (2000)

    (a) D. A. M. "Density matrix theory of quantum dynamics in an active medium: photodesorption of diatomics"

    (b) D. A. M. "First principles collision dynamics of electronic energy and charge transfer"

245. Invited paper D.A.M. "First principles dynamics of many-electron atom-atom collisions", Symposium on "Novel Computational Approaches to Low-Energy Atom Scattering", UF, Feb. 3, 2001.

246. Three contributed papers, 2001 Pan-American Workshop on Molecular and Materails Sciences: Theoretical and Computational Aspects", Univ. of Florida, February 21-23, 2001:

    (a) A. Reyes, K. Runge, and D. A. M. "Alkali-rare gas atom interactions from a first principles dynamics using effective atomic core potentials"

(b) A. Santana-Vargas, and D. A. M. "Density matrix treatment of nonlinear optical response of CO/Cu(001): Photodesorption yields"

(c) B. Thorndyke and D. A. M. "Using the Wigner transform in quantum/classical simulations"

247. Three contributed papers, Sanibel International Symposia, St. Augustine, Florida, February 24-March 2, 2001:

(a) A. Reyes, K. Runge, and D. A. M. "First principles dynamics of alkali atom rare-gas atom interactions using effective atomic core potentials"

(b) A. Santana-Vargas, and D. A. M. "Nonlinear optical response and chirping effects in photodesorption: Density matrix treatment of CO/Cu(001)"

(c) B. Thorndyke and D. A. M. "Density matrix approach to the time-resolved spectra of alkali atoms in rare gas clusters"

248. Invited paper, D. A. M. "Nonlinear yields of diatomics photodesorbed from metals by femtosecond pulses: a density matrix treatment" Harvard-Smithsonian ITAMP Workshop, June 14-16, 2001

249. Contributed paper, A. Reyes, K. Runge, and D.A.M. "First principles dynamics of alkali atom rare-gas atom interactions using effective atomic core potentials", Coulson Summer School, Oxford, England, Aug. 15-25, 2001.

250. Invited paper, D. A. M. "Density matrix treatment of collision- and photo-induced electronic energy and charge transfer", National Amer. Chem. Soc. meeting, Chicago, August 26-30, 2001.

251. Two contributed papers, Sanibel International Symposia, St. Augustine, Florida, February 23-March 1, 2002:

(a) A. Reyes, and D. A. M. "First principles dynamics of electronic excitation and polarization in alkali-rare gas atom interactions"

(b) A. B. Pacheco and D. A. M. "Electronic state-to-state collision cross sections using transition integrals"

252. Two contributed papers, "Celebration of Chemistry" Conference, UF, March 11, 2002:

(a) A. Reyes, and D. A. M. "First principles dynamics of electronic excitation and polarization in alkali-rare gas atom interactions"

(b) A. B. Pacheco and D. A. M. "Electronic state-to-state collision cross sections using transition integrals"

253. Three contributed papers, American Chemical Society National Meeting, Orlando, Florida, April 7-11, 2002:

    (a) A. Reyes, D. A. M., and B. Thorndyke "Electronic excitation, polarization, and light emission in alkali-rare-gas atom interactions from a first principles dynamics"

    (b) A. Santana-Vargas, and D. A. M. "Effect of adsorbate vibrational motions on the nonlinear photodesorption yields for CO/Cu(001)"

    (c) B. Thorndyke, D. A. M., and A. Reyes "Dynamics of alkali atoms in clusters: Density matrix theory and quantal/classical coupling"

254. Invited paper, D. A. M. "Eikonal methods for quantum molecular dynamics in configuration and phase space" Harvard-Smithsonian Inst. Theoretical At. Mol. Physics Workshop, May 9-11, 2002

255. Seminar Talk D. A. M. Univ. of Florida QTP, Oct. 30, 2002, "Dissipative quantum molecular dynamics at surfaces and in clusters"

256. Invited paper, D. A. M. "Dissipative dynamics of femtosecond desorption: CO/Cu(001)", ACS South East Regional Meeting, S. Carolina, November 13-16, 2002.

257. Two contributed papers, Sanibel International Symposia, St. Augustine, Florida, February 22-March 1, 2003:

    (a) A. Reyes, D. A. M., and A Pacheco "First principles quantum dynamics of electronic excitation and spin-orbit recoupling in alkali-noble gas atom interactions"

    (b) A. Santana and D. A. M. "Density matrix treatment of dissipative photodesorption: Adsorbate vibrational motions and chirping effects for CO/Cu(001)"

258. Invited paper, Pan-American Workshop, Cuernavaca, Mexico, Feb. 17-19, 2003, D.A.M. "Dissipative quantum dynamics at surfaces and in clusters"

259. Invited oral presentation, Amer. Chem. Soc. National Meeting, New Orleans March 23-27, 2003, D. A. M. and A. Santana, "Time propagation of the density matrix for dissipative dynamics: Photodesorption by femtosecond pulses"

260. Contributed paper, Amer. Phys. Soc. DAMOP meeting, Boulder CO, May 21-24, 2003, A. Reyes, D. A. M. and A. Pacheco "Electronic excitation and spin-orbit recoupling cross sections for alkali-atom/noble gas-atom collisions from a first principles quantum dynamics"

261. Invited paper, II Intern. Conf. on Elementary Processes in Molecule-Metal Surface Interactions, May 3-8, 2003, San Juan, Puerto Rico, A. Santana and D. A. M. "Femtosecond photodesorption of CO from Cu(001)"

262. Contributed paper, Celebration of Research, Chemistry Department Meeting, University of Florida, December 8, 2003, A. B. Pacheco, A. Reyes, B. Thorndyke and D.A.M. "Alkali atom-noble gas atom interactions: From atom-atom collisions to optical spectra in solvents"

263. Three contributed papers, Sanibel International Symposia, St. Augustine, Florida, February 28-March 5, 2004:

    (a) A. B. Pacheco and D.A.M. "Dynamics of light emission during alkali atom-noble gas atom interactions: From atom-atom collisions to interactions in clusters"

    (b) B. Thorndyke and D. A. M. "Mixed Quantum/Classical Dynamics of Electronically Excited Molecular Systems: A Model of Near Resonant Electron Transfer"

    (c) A. Leathers and D.A.M. "Numerical method for the integration of the density matrix for non-Markovian dissipative molecular dynamics"

264. Contributed paper, American Phys. Soc. March 2004 Meeting, Montreal, Canada, B. Thorndyke and D. A. M. "Mixed Quantum/Classical Dynamics of Electronically Excited Molecular Systems: A Model of Near Resonant Electron Transfer"

265. Invited paper, American Chemical Society National Meeting, March 28-April 1, 2004, Anaheim, CA, D.A.M., A. Reyes, A. Pacheco, and B. Thorndyke "Time-propagation of the quantum-classical density matrix for electronically excited molecular systems"

266. Seminar, IMAFF, Consejo Superior de Investigaciones Cientificas, Madrid, Spain, May 10, 2004 "The quantum-classical density matrix for electronically excited molecular systems"

267. Seminar, Chemistry Department, Strasbourg University, France, May 25, 2004 "First principles dynamics of electronically excited systems"

268. Seminar, Chemistry Department, Ecole Normale Superieure, Paris, France, May 26, 2004, "Propagation of the quantum-classical density matrix for electronically excited molecular systems"

269. Presentation, University of Florida Office of Research, Energy Colloquium, November 1, 2004, "Modeling photoinduced molecular kinetics at surfaces"

270. Three contributed papers, Sanibel International Symposia, St. Simons Island, Georgia, March 6-11, 2005:

    (a) A. B. Pacheco and D.A.M. "Dynamics of light emission during alkali atom-noble gas atom interactions: From atom-atom collisions to interactions in clusters"

(b) A. Leathers and D.A.M. "Calculation of the density matrix for the non-Markovian dissipative dynamics of adsorbates on metal surfaces"

271. Invited paper, American Chemical Society National Meeting, March 13-17, 2005, San Diego, CA, D.A.M., A. Santana, A. Leathers, A Sudhyadhom, and J-L. Vega "Modeling the electronics and dissipative dynamics of excited diatomics at metal surfaces"

272. Invited paper, 20th Werner Brandt Workshop, April 10-13, 2005, Univ. of Florida, Ganiesville FL, D. A. M. , A. Leathers, J-L. Vega, and S. Miret Artes "Temperature Dependence of Collisional Line Shapes: A Density Matrix Treatment"

273. Invited paper, Workshop on the Quantum Dynamics of Complex Molecular Systems, Paris, France, May 18-20 (2005) D. A. M., B. Thorndyke, and A. Leathers "Density Matrix Treatment of Electronically Excited Molecular Systems: Applications to Cluster and Surface Dynamics"

274. Invited Paper, Sanibel Symposium, St Simons Island, Feb. 26-March 3 (2006), D. A. M., A. Leathers , and B. Thorndyke "Density Matrix Treatment of Gaseous and Adsorbate Dynamics in Electronically Excited Molecular Systems"

275. Two contributed papers, Sanibel International Symposia, St. Simons Island, Georgia, February 26-March 3, 2006:

    (a) A. B. Pacheco and D.A.M. "Light emission during interactions of an excited alkali atom inside or at the surface of a noble gas cluster: a density matrix treatment"

    (b) A. Leathers and D.A.M. "Quantum-classical density matrix treatment of the photodissociation of NaI"

276. Invited Paper, American Chemical Society National Meeting, Atlanta GA, March 26-30 (2006), D. A. M., A. Leathers, A. B. Pacheco, A. Sudhyadhom, and B. R. Thorndyke "Dissipative femtosecond dynamics of electronically excited systems: A density matrix approach"

277. Contributed paper, Sanibel International Symposia, St. Simons Island, Georgia, February 22-27, 2007, A. Leathers and D. A. M., "Density matrix treatment of combined instantaneous and delayed dissipation for an excited molecule in a medium"

278. Invited paper, American Chemical Society National Meeting, Chicago, IL, March 25-29 (2007), D. A. M. and A. Leathers, "Photoexcitation and electron transfer in quantum dots at surfaces: A density matrix treatment of their dissipative dynamics"

279. Contributed paper, Paris Research Center Workshop on "Energy flow dynamics in biomaterial systems", October 2-5, 2007, A. S. Leathers and D. A. M. "Numerical treatment of the reduced density matrix equations for combined instantaneous and delayed dissipations in many-atom systems"

280. Contributed paper, SEP 2007 Workshop, Center for Nonlinear Studies, Los Alamos National Lab, Santa Fe, New Mexico, October 1-4, 2007, D. S. Kilin and D. A. Micha "Ab initio treatment of surface photovoltaic effects at semiconductors"

281. Invited paper, 2007 Pan-American Workshop on Molecular and Materials Sciences", Cuernavaca, Mexico, October 9-11, 2007, "Photoinduced phenomena at solid surfaces: Density matrix treatment of the dissipative dynamics"

282. Invited paper, American Chemical Society National Meeting, New Orleans, LO, April 6-10 (2008), D. A. M., A. S. Leathers, and D. S. Kilin "Rates of quantum state population and coherence relaxation during optical excitation of surfaces: A density matrix computational approach"

283. Contributed paper, American Chemical Society National Meeting, New Orleans, LO, April 6-10 (2008), D. S. Kilin, and D. A. Micha "Quantum chemical calculations of surface photovoltages: Applications to adsorbates on Si(111)"

284. Invited paper, Institute for Mathematics and its Applications, 2008-2009 Program on Mathematics and Chemistry, workshop on coherence, control, and dissipation, Minneapolis, Minn., March 2008, title to be announced.

RESEARCH PROGRAM

General Areas of Research

My general interests are the theoretical and computational aspects of molecular and materials sciences, with an emphasis on the unified treatment of physical and chemical kinetics using quantum molecular dynamics. In particular:

- Theoretical methods for the many-electron description of time-dependent molecular phenomena, few-body and many-body theory of molecular collisions, and density matrix theory of molecular response and rate processes. Applications of interest relate to energy transfer, electron transfer and reactions in molecular collisions, intermolecular forces, gas-surface interactions, cluster dynamics, photodissociation, and spectra and dynamics of adsorbates at solid surfaces.

- Computational methods for the differential and integral equations of scattering, and variational methods for scattering and time-dependent states. Path integral and wavepacket propagation in quantum dynamics, constrained simulated annealing and molecular dynamics. Algebraic and density matrix propagation methods for rate processes including dissipative phenomena. Integration of stochastic differential equations for coupled quantal and classical degrees of freedom, and of differential equations for coupled fast and slow degrees of freedom. Expansions in travelling atomic basis functions for time-dependent many-electron states.

- Computer visualization and animation of molecular interactions. Temporal evolution of both nuclear motions and electronic densities. Animation of electronic transitions involving time-dependent molecular orbitals.

Ongoing Research and Its Continuation in the Near Future

Studies presently being carried out with research assistants and associates include:

- Optical properties of solid surfaces and nanostructured adsorbates on surfaces, relevant to capture and conversion of solar energy. In particular, adsorbed clusters on semiconductor surfaces.

- Time-dependent molecular orbital and many-electron theory and its application to electronic rearrangement in atomic collisions. Electronic energy and charge transfer, and orbital polarization, in collisions of ions with atoms and diatomics. Time-dependence of light emission and of spin-orbit recoupling.

- Scattering by solid surfaces, particularly of ions and fast neutral atoms by metal surfaces. Energy transfer in the scattering of atoms by diatomic adsorbates, leading to adsorbate vibrations. Electron transfer in the scattering of alkali ions by metal surfaces of W, Ni and Cu. Calculation of cross sections for neutralization and for orbital polarization.

- Photodesorption by visible and UV radiation of molecules adsorbed on metal surfaces of Ni and Cu metals; calculation of line shapes in steady-state experiments, and of lifetimes and yields in pulsed light experiments. This is being done within density matrix theory, developing computational methods suitable for dissipative dynamics in extended systems.

- Spectra of atoms and molecules in atomic clusters. Isomerization dynamics of atomic clusters of transition metal ions and rare gas atoms.

- Molecular rearrangement involving electronic transition in collisions of hydrogen, alkali and alkali-earth atoms with atoms and diatomics, and photodissociation of halide compounds, in terms of self-consistent eikonal methods.

- Visualization and animation of collisional electron transfer, and of photodesorption. Animation of light emission during atomic collisions.

Work planned in the near future involves density matrix theory and computational methods for extended molecular systems with stochastic forces, particularly as it relates to phenomena at surfaces and to electronically excited atoms and molecules in clusters; scattering of atoms and ions by molecular adsorbates on solid surfaces using collisional time-correlation functions; and generalizations of time-dependent Hartree-Fock theory designed to provide a quantitative theory of molecular rearrangement.

Long-Range Plans

We foresee continuing work to unify physical and chemical kinetics in the gas phase, in clusters, and at the gas-solid interface using methods based on density matrix theory. This aims to provide a truly fundamental approach to chemical dynamics, where electronic and nuclear motions are considered together to account, for example, for quantum state correlations and selection rules in dynamical phenomena and quantum control of reaction rates. It includes the study of dissipative and cooperative processes in condensed phases and at interfaces. A related aim is to extend present computational methods of molecular dynamics to include quantum effects, and to develop a library of computer programs to do classical and quantum molecular dynamics calculations.