

Curriculum Vitæ

Nils Yngve Öhrn

U.S. Citizen; Married to Ann M. M. Thorsell; Two daughters, Elisabeth and Maria, one granddaughter, Katarina.

Education

- F. M. (M. S.) Uppsala University, Sweden-1958.
- F. L. (Ph. D.) Uppsala University, Sweden-1963.
- F. D. (D. Sc.) Uppsala University, Sweden-1966.

Professional Record

- Professor of Chemistry and Physics, University of Florida, Gainesville, 1971-present.
- Director, Quantum Theory Project, University of Florida, 1983-1998.
- Visiting Professor, H.C. Ørsted Institute, Copenhagen University, Copenhagen, Denmark, Oct.-Dec. 1995.
- Chairman, Department of Chemistry, University of Florida, 1977-1983.
- Visiting Professor of Chemistry, University of Utah, Salt Lake City, Utah, Fall, 1981, and Fall, 1984.
- Associate Director, Quantum Theory Project, University of Florida, 1967-1977.
- Visiting Professor of Chemistry, Aarhus University, Denmark, 1970-1971.
- Associate Professor of Chemistry and Physics, University of Florida, Gainesville, 1966-1970.
- Research Associate, Uppsala University, Sweden, 1963-1966.

- Visiting Assistant Research Professor, Department of Chemistry, University of Florida, Gainesville, 1961-1963.
- Research Assistant, Quantum Chemistry Group, Uppsala University, Sweden, 1958-1961.

Present Research Interests

Development of theoretical and computational methods applying quantum mechanics and statistical mechanics to atomic and molecular processes, in particular the electronic structure and reaction dynamics of molecular systems. Development and application of rigorous and computationally feasible time-dependent theoretical methods in study of transition probabilities, cross sections, and rates of processes, such as charge transfer, energy loss, bond breaking and bond formation, at the atomic and molecular level. Development and application of rigorous, computationally feasible theoretical methods in the study of spectra and properties of matter particularly with the use of many-body and propagator theory.

Membership in Professional Societies

- Fellow of the American Physical Society.
- Member of the American Chemical Society.

Honorary Societies and Foreign Academies

- Sigma Xi
- Phi Beta Kappa
- Royal Academy of Sciences, Uppsala University, Sweden
- Finnish Academy of Sciences
- Royal Danish Academy of Sciences and Letters

Awards and Recognitions

- Fulbright-Hays Fellow, 1961-1963.
- Gold Medal awarded by The King of Sweden , March, 1980, for furthering cultural and scientific relations between Sweden and the United States of America.
- The Florida Academy of Sciences Medal, 1984.
- Danish Research Academy Lecturer at Aarhus University, Denmark Fall Semester 1991, and Summer Term 1992.
- The "Chaire Francqui Interuniversitaires d'Etranger" in Belgium (the Universities of Namur, Antwerp, and Liege) April-September 1995.
- Teaching Improvement Program (TIP) Award at the University of Florida 1995.
- The 1997 American Chemistry Society Florida Award.
- Professional Excellence Program (PEP) Award at the University of Florida, 1998.
- Danish Research Academy Lecturer at Aarhus University, Denmark, Fall Semester 1999.
- Advances in Quantum Chemistry, Vol **35**, Academic Press (1999) entitled "Propagating Insight: A Tribute to Yngve Öhrn" (Eds. John R. Sabin, Michael C. Zerner, J. Vincent Ortiz, and Henry Kurtz)
- The University of Florida Teacher/Scholar of the Year 2003/2004.
- A symposium in Honor of N. Yngve Öhrn, *Quantum Molecular Response and Molecular Reaction Dynamics: Theory and Computation* an ICCMSE Highlighted Symposium, held at Corfu, Greece, September 25-30, 2007.

Current Research Grants

- NSF Sept.05-Aug.08, \$360,000

Editorial Work

- Editor-in-Chief of the International Journal of Quantum Chemistry, Interscience.
- Editor of the International Journal of Quantum Chemistry, Interscience, 1967-2000.
- Member of the Editorial Board of Chemical Physics Letters, 1987-1990.

Invited Seminars, Talks, Lectures, etc. 1976-

- "The Theory of Ionization and Excitation Processes," International Workshop, Sanibel Island, Florida, January, **1976**.
- "Propagators in Quantum Chemistry," Departmental Colloquium in the Chemistry and Physics Departments, Cornell University, Ithaca, New York, March, **1976**.
- "Methods without Wavefunctions," The 2nd International Congress on Quantum Chemistry, New Orleans, Louisiana, April, **1976**.
- Twenty Lectures on "Symmetry in Quantum Chemistry," and 10 Lectures on "Green's Function Techniques," The International Summer Institute, Uppsala University, Uppsala, Sweden, August, **1976**.
- "Propagator Calculations of Molecular Electronic Structure," Oji International Seminar, Hokkaido, Japan, September, **1976**.
- "Calculation and Theory of Photoionization Cross Sections," Sandbjerg, Denmark NATO-SCHOOL, October, **1976**.
- Two plenary lectures in the International Workshop on Quantum Chemical Methods, held on Sanibel Island, January, **1977**.
- Lecture on "Diagrammatic Techniques and the Electron Propagator," Aarhus University, Aarhus, Denmark, July, **1977**.
- Lecture on "Single-Particle Methods for Large Clusters of Atoms," Helsinki Technological University, Otaniemi, Finland, August, **1977**.

- Twenty Lectures on "Symmetry in Molecular Theory," and 10 lectures on "Propagator Methods," in the International Summer School in Quantum Chemistry, Uppsala University, Uppsala, Sweden, August, **1977**. (Sixty participants from twenty-three different nations.)
- Invited speaker in the Operation Interface Conference arranged by the American Chemical Society in New Orleans, Louisiana, November, **1977**.
- Lecture at the International Symposium on Quantum Chemistry and Solid-State Physics held at Palm Coast, Florida, March, **1978**.
- Seminar speaker Battelle Research Labs and Ohio State Chemistry Department, Columbus, Ohio, April, **1978**.
- Outside evaluator on doctoral dissertation and defense at Aarhus University, Aarhus, Denmark, May, **1978**.
- Lecturer at the NATO Advanced Study Institute of Theoretical Aspects of the Electronic Structure and Properties of the Excited State of Atoms, Molecules and Solids, on the Island of Kos, Greece, June, **1978**.
- Lecturer at the International Summer School on Quantum Chemistry at Uppsala University, Uppsala, Sweden, September, **1978**.
- Invited plenary speaker at the Nobel Symposium on Many-Body Theory of Atomic Systems at Göteborg, Sweden, June, **1979**.
- Invited plenary speaker at the Symposium on Many-Body Theoretical Approaches to Electron Correlation in Molecules, at Kobe, Japan, October **1979** (Chemical Society of Japan).
- Lecturer at the International Summer School on Quantum Chemistry at Uppsala University, Uppsala, Sweden, September **1980**.
- Session Chairman at the National Resource for Computation in Chemistry's conference on "Perturbation Methods in Quantum Chemistry," Seattle, Washington, July, **1981**.
- Lecturer at University of Namur, Namur, Belgium, August, **1981**.

- Lecturer at the International Summer School on Quantum Chemistry and Solid-State Physics at Uppsala University, Uppsala, Sweden, September, **1981**.
- Invited plenary lecture at the ACS National Meeting in Las Vegas, Nevada, March, **1982**.
- Member of an International Evaluation Committee of Applicants for a Swedish Research Council Professorship in Atomic and Molecular Physics, Stockholm, Sweden, June, **1982**. (Committee of two with Professor T. Anderson, Aarhus University, Aarhus, Denmark.)
- Invited poster lecture at the IVth International Congress on Quantum Chemistry at Uppsala, Sweden, June, **1982**.
- Member of International Evaluation Committee of Applicants for Chair in Theoretical Physics at Stockholm University, Stockholm, Sweden, July, **1982**. (Committee of three with Professor Kolos, Warsaw, Poland, and Professor R. Hoffman, Cornell University.)
- Invited lecturer at the International Summer School in Quantum Chemistry at Uppsala University, Uppsala, Sweden, August, **1982**.
- BCS lecturer at Namur University, sponsored by the Belgian Chemical Society for one week course on Propagators in Quantum Chemistry, September, **1982**.
- Member of International Evaluation Committee of Applicants for the Chair of Electron Physics (Materials Research) at the Finland Technical University, Otaniemi, Finland, October, **1982**.
- Invited lecturer at the International Summer Institute in Quantum Chemistry at Uppsala University, Uppsala, Sweden, August, **1982**.
- Invited seminar speaker at Oak Ridge National Laboratory, Oak Ridge, Tennessee, November, **1983**.
- Invited seminar speaker at Aarhus University, Aarhus, Denmark, January, **1984**.
- Invited seminar speaker at Antwerp University, Antwerp, Belgium, May, **1984**.

- Invited seminar speaker at Chalmers University, Göteborg, Sweden, May, **1984**.
- Plenary speaker at the Nordic Molecular Physics Days, Svendborg, Denmark, May, **1984**.
- Invited seminar speaker at Bergen University, Bergen, Norway, June, **1984**.
- Invited speaker at the National ACS meeting in Philadelphia, Pennsylvania, August, **1984**.
- Invited lecturer at the International Institute on New Materials at Uppsala, Sweden and Helsinki, Finland, August, **1984**.
- Invited speaker at the Nobel Laureate Symposium on Applied Quantum Chemistry, PACCHEM 84, Honolulu, Hawaii, December, **1984**.
- Invited lecturer at the 25th Sanibel Symposium, Marineland, Florida, March, **1985**.
- Invited lecturer at the Coleman Symposium on Density Matrices at Queen's University, Ontario, Canada, August, **1985**.
- Invited speaker at the NSF-sponsored conference on the Interface of Electronic Structure and Dynamics and the Workshop on the Future of Quantum Chemistry, April, **1986**, at Snowbird, Utah.
- Invited speaker at the Saskatoon, Saskatchewan, Canada, Conference on Mathematical Chemistry, June, **1986**.
- Member of review panel of the Air Force of Scientific Research, "New Research Opportunities in Novel Propellants," March, **1986**.
- Invited speaker at the Workshop on Resonances, at Lertorpet, Sweden in August, **1987**.
- Invited seminar speaker at Aarhus University, Dept. of Chemistry, June, **1987**.
- Invited speaker at the Workshop and Symposium on Many-Body Theory at Calcutta, India, February, **1988**.

- Invited seminar speaker and ski professor at the University of Utah, Department of Chemistry, March, **1988**.
- Visiting Professor at the Department of Chemistry, Aarhus University, Aarhus, Denmark, July **1988**.
- Visiting Professor at the Department of Quantum Chemistry, University of Uppsala, August **1988**.
- Invited lecturer RUCA, University of Antwerp, Belgium. Ten lectures on Molecular Orbital Theory, June, **1989**.
- Invited lecturer at the Nordic Research Workshop on Chemical Reaction Dynamics, held at Karlskoga, Sweden, August 7-18, **1989**.
- Invited lectures: Four plenary lectures on different topics at the " Programme Gouvernemental en Technologie de l'Information Calcul de Puissance", Faculté s Universitaires Notre Dame de la Paix, Namur, Belgium, June **1990**.
- Invited lectures: "Time-Dependent Dynamics and Coherent States" (10 lectures) at the Institute of Quantum Chemistry, Uppsala University, Sweden. August-October **1990**.
- "Theory of Molecular Anions", Lecture at the Department of Chemistry, Uppsala University, Sweden. August **1990**.
- "Atom-Diatom Reactive Collisions", Department of Chemistry, Uppsala University, Sweden. September **1990**.
- "Time-Dependent Molecular Theory and Coherent States", University of Copenhagen, H.C.Ørstedt's Institute. December **1990**.
- "Introduction to Time-Dependent Theory of Molecular Processes", Aarhus University, Denmark. A series of lectures sponsored by the Danish Research Academy, June-October **1991**.
- "Theory of Time Dependence in Elementary Chemical Reactions", invited plenary lecture at the Danish Chemical Society Meeting, at Odense University, June 12, **1991**.

- "1/N expansions and Coherent States" invited lecture at the Scandinavian Workshop on Dimensional Scaling, June 16-22, **1991**, at H. C. Ørsted Institute, University of Copenhagen, Denmark.
- "Electron-Nuclear Dynamics in Molecular Systems" invited lecture at the NATO Advanced Research Workshop on Time-Dependent Molecular Dynamics: Experiment and Theory, held at Snowbird, Utah March 30- April 3, **1992**.
- Invited seminar "Time-Dependent Theory of Chemical Reactions" at H.C. Ørsted Institute, Copenhagen, Denmark. August, **1992**.
- Invited seminar "Time-Dependent Theory of Chemical Reactions" at Department of Chemistry, Aarhus University, Aarhus, Denmark, November, **1992**.
- Invited SCF lecturer at Facultes Universitaires Notre-Dame de la Paix, Namur, Belgium 10 lectures on "Theory of Spectroscopy in Terms of Propagators." May 24-29, **1993**.
- Plenary speaker at the International Symposium on Coherent States: Past, Present, and Future, June 14-17, **1993**. "A Time-Dependent Theory for Electron Nuclear Dynamics".
- Plenary speaker at the Symposium on Molecular Interactions, at Aarhus University, Aarhus, Denmark, December 10 and 11, **1993**.
- Presentation at the Swedish Defense Laboratories (FOA), December 14, **1993**.
- Plenary speaker at the 34-th annual International Sanibel Symposium, February, **1994**, at Sawgrass, FL.
- Plenary speaker at the Symposium on the Chemical Bond, July 26 and 27, **1994**, University of Copenhagen, Denmark.
- Seminar Speaker at Uppsala University, Institute of Quantum Chemistry, Feb. 10 **1995**, "Coherent States for Chemical Reactions".
- Seminar Speaker, University of Utah, Chemistry Department, "The Electron Nuclear Dynamics Theory Applied to Ion-Molecule Collisions", March 8, **1995**.

- Speaker at the Memorial Symposium for J.-L. Calais, at Uppsala University, "Electron Nuclear Dynamics", June 15, **1995**.
- First occupant of the Francqui Interuniversity Chair in Belgium (Chaire Francqui Interuniversitaires d'Etranger de Belgique) April-September **1995**. Inaugural Public Lecture June 2, "Time and Chemistry", at F.U.N.D.P., Namur. Lecture series on "Applied Group Theory" during June, July and August. Other Lectures at various Belgian Universities: Mons September 13, Leuven September 19. Antwerp, September 28, 29.
- Seminar at the Chemistry Department, Aarhus University, October 19, **1995** "Ion-molecule reactions in a time-dependent formulation".
- Final lecture in the Francqui series at F.U.N.D.P. (Namur, Belgium) on October 27, **1995** "Quantum Chemistry; An Overview and a Look to the Future".
- Visiting Professor at H. C. Ørsted Institute, Copenhagen, Denmark, October, November, December, **1995**, Lecture series about "Time-Dependent Theory of Molecular Reaction Dynamics".
- Seminar at the Chemistry Department, University of Utah, "Time-Dependent Theory of Molecular Reaction Dynamics", March 13, **1996**.
- Plenary speaker at the Workshop on Algebraic Methods in Quantum Dynamics" held at the Fields Institute, Toronto, Canada, "Coherent States in Molecular Reaction Dynamics", May 7-11, **1996**.
- Invited lecture, "Excited reagents and products in molecular collisions without potential energy surfaces" at the National ACS meeting, Orlando, August 25-29, **1996**.
- Invited lecture, "Electron Nuclear Dynamics" , at the Symposium held on the occasion of P.-O. Löwdin's 80 year birthday at Sanibel Island, October 26-29, **1996**.
- Invited Lecture, "Application of a Time-Dependent Theory to Molecular Processes" at the 5th Conference on Current Trends in Computational Chemistry, held at Vicksburg, Mississippi, November 1 and 2, **1996**.

- MDAD (Molecular Dynamics After Dark) seminar at the University of Utah, Chemistry Department, Salt Lake City, Utah, March 12, **1997**, "New results with END".
- Departmental Colloquium speaker at the Physics Department, Brigham Young University, Provo, Utah, March 13, **1997** "Molecular Reaction Dynamics".
- Award Lecture at Regional ACS Meeting, Orlando, Florida on Friday May 2, **1997**, "Electron Nuclear Reaction Dynamics".
- Invited plenary lecture at the XXth Brazilian National Conference on Condensed Matter Physics, at Caxambu, Brazil, June 10-14, **1997**.
- Invited lecture at the "Electron Correlation Workshop: Fifty years of the correlation problem.", at Cedar Key, Florida, June 15-18 **1997** "Correlation between electrons and nuclei in molecular reaction dynamics".
- Invited seminar at the Technical University of Munich, Germany on June 26, **1997**, "Energetic proton collisions with methane and water".
- Invited lecture to the Society of Physics Students at the University of Florida, October 15, **1997** "Reactive Molecular Collisions".
- Departmental Colloquium speaker at the Department of Chemistry, Aarhus University, Denmark, November 24, **1997** "A Time-Dependent Picture of Molecular Reaction Dynamics".
- Featured speaker at the meeting of the Royal Danish Academy of Science and Letters at Copenhagen, Denmark, November 27, **1997** "The Concept of Time in Chemistry".
- Invited speaker at the Symposium on Adiabatic and Nonadiabatic Molecular Dynamics at Uppsala University, Sweden, December 18, **1997** "The Electron Nuclear Dynamics Theory".
- Invited speaker at the Frank E. Harris Symposium, held in Park City, Utah, February 21, **1998** "Fragmentation ratios in reactive collisions of protons with methane molecules".

- Invited seminar at the Faculté Universitaires Notre Dame de la Paix, Namur, Belgium, June 12, **1998**, "Molecular reaction dynamics without potential energy surfaces".
- QTP seminar, University of Florida, Nov. 18 **1998**, "How to get out of the adiabatic straitjacket".
- Invited seminar at the Chemistry Department, Aarhus University, Denmark, December 16, **1998**, "New results in molecular reaction dynamics".
- Invited talk at the workshop on Time-Dependent Quantum Molecular Dynamics held at Brian Head, Utah, March 13-17, **1999**, "Electron Nuclear Dynamics of Reactive Molecular Collisions."
- Series of lectures on "Molecular Reaction Dynamics" at Aarhus University, Denmark, Fall Semester **1999**.
- Lecture on "Chemistry career in the USA" at Workshop for the Center for Metal Catalyzed Reactions, Aarhus University held at Svinklöv Badehotel, September 14-15, **1999**.
- Seminar at the Department of Physics, Aarhus University, Denmark, "Ion Atom Collisions in the keV Range", September 23, **1999**.
- Lecture at the Symposium "Synergism between experiment and theory in organic chemistry" honoring Professor Göran Bergson, held at Uppsala University, Uppsala, Sweden, October 1, **1999**; "Fragmentation of methane by collisions with 30 eV protons".
- The Chair's Invitational Seminar, "Time and Chemistry" at the University of Florida Chemistry Department on April 21, **2000**.
- Plenary lecture at DYNAM 2000 in Arcachon, France, " $D_2 + NH_3^+$ " May 31-June 3, **2000**.
- Seminar at the Department of Chemistry, University of Copenhagen, Denmark, August 15, **2000**, "Electron Nuclear Dynamics, Recent Progress".
- Invited plenary lecture "Abstraction and exchange mechanisms of the $D_2 + NH_3^+$ reaction; Application of the END theory", at the MOLEC conference September 17-22, **2000** in Jerusalem, Israel.

- Invited lecture tour of Indian institutions in December **2000**: Dec. 6 at IIT, Bombay: "Nonadiabatic theory of molecular reaction dynamics"; Dec. 7: Tata Institute for Fundamental Research: "Electron Nuclear Dynamics"; Dec. 11: National Chemistry Laboratory, Pune: "Electron Nuclear Dynamics"; Dec. 13: Indian Institute of Science, Bangalore: "Nonadiabatic theory of molecular reaction dynamics"; Dec. 15: Theoretical Physics Institute of Mathematical Sciences, Madras(Chennai): "Nonadiabatic treatment of ion-atom, and ion-molecule collisions". Dec. 19: Jawahrlal Nerhu University, Delhi: "Electron Nuclear Dynamics".
- Invited plenary lecture at the Indian Theoretical Chemistry Conference at IIT, Kanpur, Dec. 22, **2000**: "Electron Nuclear Dynamics".
- Invited plenary lecture in the one-day conference on "Novel computational Approaches to Low-energy Atom-Atom and Atom-Ion Scattering" held at the University of Florida, Feb. 3, **2001**.
- Invited plenary speaker at the National ACS Meeting in Chicago, August 26-30, **2001**, Symposium on "*Ab initio* simulation of chemical dynamics".
- Invited plenary speaker at the Regional ACS Meeting in Savannah, Georgia, September 23-26, **2001**, Symposium on "Interaction between *ab initio* computations and experiment".
- Invited Physics Departmental Seminar, University of Florida, October 18, **2001** "Direct Nonadiabatic Dynamics of Molecular Processes".
- Invited to deliver the Charles A. Coulson lecture at the University of Georgia, April 16, **2002**.
- Invited lecturer at the International Seminar and Workshop on "Quantum Dynamical Concepts: From Diatomics to Biomolecules", at Max-Planck-Institut für Physik Komplexer Systeme, Dresden, Germany, April 15- May 3, **2002**.
- Invited lecturer at the ITAM Workshop on "Computational Approaches to Time-Dependent Quantum Dynamics" at the Harvard-Smithsonian Observatory, May 9-11, **2002**.

- Invited plenary speaker ("Electron Nuclear Dynamics") at the IV-th International Congress of Theoretical Chemical Physics, Marly-le-Roi, Paris, France, July 9-16, **2002**.
- Invited speaker ("Proton collisions with organic molecules") at WATOC 2002, Lugano, Switzerland August 4-10, **2002**.
- Invited seminars ("Direct nonadiabatic molecular reaction dynamics") at the Institute of Quantum Chemistry, Uppsala University, Sweden, November 4 and 6, **2002**.
- Invited talk ("Direct nonadiabatic molecular reaction dynamics") at SERMACS 02 in Charleston, SC November 14-15, **2002**.
- Invited seminar at the Department of Chemistry, Aarhus University, Denmark, May 8, **2003**: "Recent Results with Electron Nuclear Dynamics Theory"
- Invited plenary lecture at the Werner Brandt Workshop, Playa del Carmen, Mexico, June 5, **2003**: "Direct, Nonadiabatic, Molecular Collision Theory".
- Invited plenary lecture to the G. D. Billing memorial symposium at Copenhagen University, Copenhagen, Denmark, August 11-13, **2003** "Direct, Nonadiabatic, Molecular Reaction Dynamics".
- Invited seminar at the department of Physics, Kansas State University, Manhattan, Kansas, October 8, **2003**.
- The H. H. King Lecturer at Kansas State University, Manhattan, Kansas on October 9, **2003**.
- Symposium at Georgia Tech on the occasion of Professor Jean-Marie André's 60'th birthday: Speakers: Enrico Clementi, H. F Schaefer, and Y. Öhrn: "Chemistry with Classical Nuclei and Quantum Electrons", April 5, **2004**.
- Conference on "Response Theory and Molecular Properties" at Sandbjerg Estate, Denmark, May 5-8, **2004**. Lectures by Y. Öhrn: "Jan Linderberg, Scientist, Teacher, Friend" and "Time-Dependent Molecular Reaction Dynamics".

- Invited lectures at the Workshop on "Nonadiabatic Molecular Dynamics" at Telluride, Colorado, August 1-6, **2004**.
- Invited lecture at the 25th Brandt-Ritchie Workshop on Particle Penetration Phenomena and Excitations of Solids, in Gainesville, FL April 10-13, **2005**. "Direct, Nonadiabatic Molecular Reaction Dynamics"
- Invited lecture in the Workshop on "Quantum Dynamics of Complex Molecular Systems", in Paris, France, May 18-21, **2005**.
- Invited lecture at the University of Stockholm, AlbaNova University Center, Monday, August 22, **2005**; "Time-dependent, direct, nonadiabatic atomic and molecular reaction dynamics".
- Invited lecture at the Workshop on "Prospects for Theory, Computation, and Simulation in the Molecular Sciences in the 21'st Century", at Spiterstulen, Norway, August 2-7, **2006**.
- Invited speaker at the Conference on Current Trends in Computational Chemistry on November 3-4 **2006** at Jackson, Mississippi.
- Invited speaker and chair at the First International Meeting on Recent Developments in the Study of Radiation Effects in Matter, Playa del Carmen, Q. Roo, Mexico, December 5-8, **2006**.
- Invited speaker at the Symposium in Honor of Professor William A. Lester, University of California, Berkeley, March 28-31, **2007**.
- Invited lecturer at the Summer School on Multiscale Simulation and Modeling, at Stockholm, Sweden, June 4-15, **2007**.
- Principal speaker at the Symposium on "Quantum Molecular Response and Reaction Dynamics; Theory and Computations" in Honor of Yngve Öhrn and part of the ICCMSE meeting at Corfu, Greece, September 25-September30, **2007**.
- Invited speaker at the SWTCC at Texas A&M, College Station, TX October 12-14, **2007**.
- Invited speaker at the Brazilian Theoretical Chemistry Conference at Poços de Caldas (MG) near São Paulo and Rio de Janeiro, Brazil November 18-21, **2007**.

Publications

1. Y. Öhrn and J. Nordling, "On the Calculation of Some Atomic Integrals containing Functions of r_{12} , r_{13} , r_{23} ," *J. Chem. Phys.* **39**, 1864 (1963).
2. C. Reid and Y. Öhrn, "On the Calculation of Real Wave Functions in Natural form for Two-Electron Systems," *Rev. Mod. Phys.* **35**, 445 (1963).
3. A. Fröman, J. Linderberg and Y. Öhrn, "Penetration Effects in the 2F -Series of CSI," *J. Opt. Soc. Am.* **54**, 1064 (1964).
4. J. Linderberg and Y. Öhrn, "Improved Single Particle Propagators in the Theory of Conjugated Systems," *Proc. Roy. Soc.* **A285**, 445 (1965).
5. Y. Öhrn and J. Linderberg, "Propagators for Alternant Hydrocarbon Molecules," *Phys. Rev.* **139**, A1063 (1965). Reprinted in the "Series of Selected Papers in Physics," by the Physical Society of Japan, *Theory of Molecular Structure II*, 131 (1966).
6. Y. Öhrn and R. McWeeny, "Justification of the One-Body Model for an Electron Outside a 'Core' with Applications to Lithium and Sodium," *Arkiv Fysik* **31**, 561 (1966).
7. Y. Öhrn and J. Nordling, "Correlated Wave Functions of the Three Electron Ions," *Arkiv Fysik* **31**, 471 (1966).
8. Y. Öhrn, "Quantum Mechanical Studies of Electronic Spectra of Atomic and π -Electron Systems," *Acta Universitatis Upsaliensis* **68**, (1966).
9. Y. Öhrn and J.L. Calais, "Approximations in Quantum Chemistry," *Sv. Kem. Tidskr.* **79:4**, 229 (1967).
10. O. Mårtensson and Y. Öhrn, "Complex Hybridization of Orbitals of s and p Type," *Theor. Chim. Acta (Berl)* **9**, 133 (1967).
11. J. Linderberg and Y. Öhrn, "Improved Decoupling Procedure for Green Functions," *Chem. Phys. Letters* **1**, 295 (1967).
12. R. Manne and Y. Öhrn, "Chemistry Graduate Education in Sweden and USA," *Sv. Kem. Tidskr.* **79**, 11 (1967).

13. J. Linderberg and Y. Öhrn, "Derivation and Analysis of the Pariser-Parr-Pople Model," *J. Chem. Phys.* **49**, 716 (1968).
14. Y. Öhrn and J. Linderberg, "A Recurrence Relation for Density Matrices," Report of the Density Matrix Seminar, Queen's University, Kingston, Ontario Canada, July 1968.
15. O. Goscinski and Y. Öhrn, "Coupling of Equivalent Particles in a Field of Given Symmetry," *Int. J. Quant. Chem.* **II**, 845 (1968).
16. J. Linderberg and Y. Öhrn, "Tight Binding Model for Energy Bands in Solids," *Chem. Phys. Letters* **3**, 119 (1969).
17. J. Kouba and Y. Öhrn, "On the Projection of Many-Electron Spin Eigenstates," *Int. J. Quant. Chem.* **3**, 513 (1969).
18. J. Kouba and Y. Öhrn, "Natural Orbital Valence Shell CI-Studies of Diatomic Molecules. I. Potential Energy Curves and Spectra of Imidogen," *J. Chem. Phys.* **52**, 5387 (1970).
19. J. Gruninger, Y. Öhrn and P.O. Löwdin, "Comments on the Analysis of Atomic Correlation Energies," *J. Chem. Phys.* **52**, 5551 (1970).
20. R.J. Bartlett and Y. Öhrn, "How Quantitative is the Concept of Maximum Overlap," *Theoret. Chim. Acta.* **21**, 215 (1971).
21. S. Abdulnur and Y. Öhrn, "Calculation of Bound to Dispersion Energies," *Chem. Phys. Letters* **6**, 502 (1970).
22. J. Kouba and Y. Öhrn, "Natural Orbital Valence Shell CI-Studies of Diatomic Molecules. II. Potential Energy Curves and Spectra Boron Carbide," *J. Chem. Phys.* **53**, 3923 (1970).
23. J. Kouba and Y. Öhrn, "Natural Orbital Iterations for the Ground State of Nitric Oxide," *Int. J. Quant. Chem.* **5**, 539 (1971).
24. P.W. Thulstrup, Y. Öhrn and J. Linderberg, "Hall's Variational Principle for Excited States," *Chem. Phys. Letters* **9**, 488 (1971).
25. S. F. Abdulnur, J. Linderberg, Y. Öhrn and P. W. Thulstrup, "Atomic Central Field Models for Open Shells with Application to Transition Metals," *Phys. Rev.* **6**, 889 (1972).

26. E.W. Thulstrup and Y. Öhrn, "Configuration Interaction Studies of NO and NO⁺ with Comparisons to Photoelectron Spectra," *J. Chem. Phys.* **37**, 3716 (1972).
27. A. Andersen and Y. Öhrn, "Configuration Interaction Studies of NF and NF⁺," *J. Mole. Spectr.* **45**, 358 (1973).
28. P. Jørgensen and Y. Öhrn, "Triplet-Triplet Absorption Spectra of Alternant Hydrocarbons within the Grand Canonical Time-Dependent Hartree-Fock Approximation," *Chem. Phys. Letters* **18**, 261 (1973).
29. P. Jørgensen and Y. Öhrn, "A Comparison of Two Statistical Approaches to Calculate Atoms and Molecular Orbitals," *Phys. Rev.* **8A**, 112 (1973).
30. P. Linder, Y. Öhrn and J. Sabin "Semi-Empirical Investigation of the Electronic Structure and Stability of the Oxycumulenes," *Int. J. Quantum Chem.* **7S**, 261 (1973).
31. M. Vucelic, Y. Öhrn and J.R. Sabin, "An Vibrational and Electronic Properties of Carbon Dioxide," *J. Chem. Phys.* **59**, 3003 (1973).
32. G.D. Purvis and Y. Öhrn, "Atomic and Molecular Electronic Properties and Spectra from the Electron Propagator," *J. Chem. Phys.* **60**, 4063 (1974).
33. P.W. Thulstrup, E.W. Thulstrup, A. Andersen and Y. Öhrn, "Configuration Interaction Calculation of Some Observed States of NO⁻, NO, NO⁺ and NO⁺⁺," *J. Chem. Phys.* **60**, 3975 (1974).
34. R.L. Tyner, W.M. Jones, Y. Öhrn and J.R. Sabin, "Semi-Empirical Calculations on Phenylcarbene, Cycloheptatrienyliene and Cycloheptatetraene and their Benzo-Annulated Derivative," *J. Am. Chem. Soc.* **96**, 3765 (1974).
35. Y. Öhrn, Book Review of "Many-Body Problems, by G.E. Brown, Elsevier, New York (1972) and The Many-Body Problems in Quantum Mechanics, by N.H. March, W.H. Young and S. Sampanthar, Cambridge U.P., New York (1967)," *Physics Today*, February 1974, P. 49.

36. J.A. Smith, P. Jørgensen and Y. Öhrn, "A Limited Basis Molecular Orbital Calculation on H_2O and H_2O^+ ," *J. Chem. Phys.* **62**, 1285 (1975).
37. E-K. Viinikka and Y. Öhrn, "Ci-Studies on the Multiplet Structure of the Core Hole States in Transition Metal Ions," *Phys. Fenn. (Finland)* **9**, 304 (1974).
38. V. H. Smith and Y. Öhrn, "On a formula for electron binding energies", in *Reduced Density Operators with Applications to Physical and Chemical Systems II*, p193 (1974) Queen's Papers in Pure and Applied Mathematics, No. 40 (Ed. R. M. Erdahl).
39. G.D. Purvis and Y. Öhrn, "Electron Propagator Calculations for the Photoelectron Spectrum for Open Shell Molecules with Application to the Oxygen Molecule," *J. Chem. Phys.* **62**, 2045 (1975).
40. G.D. Purvis and Y. Öhrn, "A Comment on a Theory of Electron Affinities," *Chem. Phys. Letters* **33**, 396 (1975).
41. E-K Viinikka and Y. Öhrn, "Configuration Mixing in the 3s-Hole State of Transition Metal Ions," *Phys. Rev.* **B11**, 4168 (1975).
42. L. Tyner Redmon, G.D. Purvis and Y. Öhrn, "Higher Order Decoupling of the Electron Propagator," *J. Chem. Phys.* **63**, 5011 (1975).
43. C. Nehr Korn, G.D. Purvis and Y. Öhrn, "Hermiticity of the Superoperator Hamiltonian in Propagator Theory," *J. Chem. Phys.* **64**, 1752 (1976).
44. G.D. Purvis and Y. Öhrn, "The Transition State, the Electron Propagator and the Equation of Motion Method," *J. Chem. Phys.* **65**, 917 (1976).
45. H. Kurtz, G.D. Purvis and Y. Öhrn, "The Calculation of the Amplitudes to the Electron Propagator from a Minimal Basis CI Calculation on N_2 ," *Int. J. Quantum Chem.* **S10**, 331 (1976).
46. J. Linderberg, Y. Öhrn and P.W. Thulstrup, "Energy Weighted Maximum Overlap (EWMO) Method," in *Methods and Structure of Quantum Science*, Plenum Press **93** (1976).

47. Y. Öhrn, "Propagator Theory of Atomic and Molecular Structure," in Proceedings from the 2nd International Congress on Quantum Chemistry, Reidel, Editors R.G. Parr and B. Pullman **57** (1976).
48. J. Linderberg and Y. Öhrn, "State Vectors and Propagators; a Unified Approach," *Int. J. Quantum Chem.* **12**, 161 (1977).
49. G.D. Purvis and Y. Öhrn, "Accurate Molecular Ionization Potentials from the Electron Propagator," *Int. J. Quantum Chem.* **S11**, 359 (1977).
50. Y. Öhrn, Book reviews of "Electron Correlation in Small Molecules," and "Introduction to Electron Theory of Small Molecules," by A.C. Hurley, September issue of *Physics Today* (1977).
51. G. Born, H. Kurtz and Y. Öhrn, "Elementary Finite Order Perturbation Theory for Vertical Ionization Energies," *J. Chem. Phys.* **68**, 74 (1978).
52. H. Kurtz and Y. Öhrn, "Calculation of Electron Binding Energies," *J. Chem. Phys.* **69**, 1162 (1978).
53. G. Born and Y. Öhrn, "Alternative Inner Projections of the Superoperator Resolvent," *Int. J. Quantum Chem.* **S12**, 143 (1978).
54. Y. Öhrn and J. Linderberg, "The Consistent RPA Ground State," *Int. J. Quantum Chem.* **15**, 343 (1979).
55. G. Born and Y. Öhrn, "A Superoperator Derivation of the 2p-h TDA Equations," *Chem. Phys. Lett.* **61**, 307 (1979).
56. Y. Öhrn, "The Calculation of Atomic and Molecular Electron Binding Energies," in *Excited States in Quantum Chemistry*, Proceedings of the NATO-ASI held at Kos, Greece, Reidel Publishing Co., June 4-18, 1978, 317.
57. H. Kurtz and Y. Öhrn, "Calculation of ²p Shape Resonances in Be and Mg," *Phys. Rev.* **A19**, 43 (1979).
58. G. Born and Y. Öhrn, "Electron Propagator Theory for the Calculation of Molecular Electron Binding Energies and Photoionization Intensities," *Phys. Scripta* **21**, 378 (1980).

59. M. Mishra and Y. Öhrn, "The Full 2p-h TDA and Other Self Energy Approximants: A Comparative Investigation," *Chem. Phys. Lett.* **71**, 549 (1980).
60. Y. Öhrn, "Electron Propagator Calculations of Molecular Electron Binding Energies," Proceedings of the Symposium on Many-Body Theoretical Approaches to Electron Correlation in Molecules at Kobe, Japan (1979).
61. J.V. Ortiz B. and Y. Öhrn, "Electron Propagator Theory of Molecular Anions," *J. Chem. Phys.* **72**, 5744 (1980).
62. M. Mishra and Y. Öhrn, "Correlated Treatment of Photoionization Cross-Sections in the Orthogonalized Plane Wave Approximation for the Ejected Electron," *Int. J. Quantum Chem.* **S14**, 335 (1980).
63. Y. Öhrn and G. Born, "Molecular Electron Propagator Theory and Calculations," in *Advances in Quantum Chemistry*, P.-O. Löwdin, Ed., Vol. **13**, 1981.
64. J.V. Ortiz B. and Y. Öhrn, "Electron Propagator Calculations of Molecular Electron Affinities," *Chem. Phys. Lett.* **77**, 548 (1981).
65. M. Mishra, P. Froelich and Y. Öhrn, "The Dilated Electron Propagator: A Bi-Orthogonal Approach," *Chem. Phys. Lett.* **81**, 339 (1981).
66. M. Mishra, Y. Öhrn and P. Froelich, "Self-Consistent Field Theory of Dilated Atomic Hamiltonians: Some Remarks," *Phys. Lett.* **84A**, 4 (1981).
67. R.L. Lozes, B. Weiner and Y. Öhrn, "Invariance Transformations and AGP Optimization," *Int. J. Quantum Chem.* **S15**, 129 (1981).
68. J.V. Ortiz, B. Weiner and Y. Öhrn, "The AGP Wavefunction and Its Relation to Other Descriptions of Electronic Structure," *Int. J. Quantum Chem.* **S15**, 113 (1981).
69. H.J. Jensen, B. Weiner, J.V. Ortiz and Y. Öhrn, "Powerful Procedure for Optimizing AGP States," *Int. J. Quantum Chem.* **S16**, 615 (1982).

70. H.J. Jensen, B. Weiner and Y. Öhrn, "AGP Propagator Calculation," Proceedings of the IVth International Congress on Quantum Chemistry, *Int. J. Quantum Chem.* **23**, 66 (1982).
71. M. Mishra, O. Goscinski, and Y. Öhrn, "Application of the second order dilated electron propagator to the treatment of Auger and shape resonances in Be" *J. Chem. Phys.* **79**, 5505 (1983).
72. M. Mishra, O. Goscinski and Y. Öhrn, "Numerical Study of the Bi-Variational SCF Method as a Zeroth-Order Dilated Electron Propagator," *J. Chem. Phys.* **79**, 5494 (1983).
73. M. Mishra, H.A. Kurtz, O. Goscinski and Y. Öhrn, "Treatment of Resonances with the Dilated Electron Propagator: The P Shape Resonance in e-Mg Scattering," *J. Chem. Phys.* **79**, 1896 (1983).
74. Y. Öhrn and J. Linderberg, "Hyperspherical Coordinates in Four Particle Systems," *Molecular Physics* **49**, 53 (1983).
75. Y. Öhrn, Book Review of "Field Theoretical Methods in Chemical Physics," by R. Paul, Elsevier Scientific Publishing Co. (1982).
76. J.V. Ortiz, R. Basu and Y. Öhrn, "Electron Propagator Calculations with a Transition Operator Reference," *Chem. Phys. Letters* **103**, 29 (1983).
77. B. Weiner, H.J. Jensen and Y. Öhrn, "Polarization Propagator Calculations with an AGP Reference State," *J. Chem. Phys.* **80**, 2009 (1984).
78. B. Weiner and Y. Öhrn, "A note on the Radiative Lifetimes of the $B^3\pi_g$ State of N_2 ," *J. Chem. Phys.* **80**, 5866 (1984).
79. M. Mishra, J. Linderberg and Y. Öhrn, "Characterization of Adiabatic States in Triatomic Collisions," *Chem. Phys. Letters* **111**, 439 (1984).
80. B. Weiner, W.D. Edwards, M. Zerner and Y. Öhrn, "Semiempirical AGP Calculations for Molecular Spectra," *Int. J. Quantum Chem.* **S18**, 507 (1984).
81. J. Linderberg and Y. Öhrn, "Kinetic Energy Functional in Hyperspherical Coordinates," *Int. J. Quantum Chem.* **27**, 273 (1985).

82. E. Deumens, L. Lathouwers, P. Van Leuven and Y. Öhrn, "The Generator Coordinate Approximation for H_2^+ ," *Int. J. Quantum Chem.* **S18**, 339 (1985).
83. H.A. Kurtz, B. Weiner, and Y. Öhrn, "Theory and Calculations on Small Molecules Using Propagator Methods with an AGP Reference," in *Comparison of Ab-Initio Calculation with Experiment: State of the Art*, Reidel Dordrecht (the Netherlands) 1985, Editor, R.J. Bartlett.
84. B. Weiner and Y. Öhrn, "Calculation of Spectroscopic Properties of the Ground and Excited State of Be_2 According to the Antisymmetrized Geminal Power Based Excitation Propagator," *J. Chem. Phys.* **83**, 2965 (1985).
85. Y. Öhrn, "The AGP-Based Polarization Propagator," *Int. J. Quantum Chem.* **S19**, 39 (1986); Erratum, *IJQC* **30**, 445 (1986).
86. E. Deumens, Y. Öhrn, L. Lathouwers and P. Van Leuven, "Applications of the Generator Coordinate Approximations to Diatomic Systems: I. The Hydrogen Molecular Ion," *J. Chem. Phys.* **84**, 3944 (1986); Erratum: *ibid.* **85**, 3138 (1986).
87. E. Deumens, B. Weiner and Y. Öhrn, "Time Dependent Antisymmetrized Geminal Power Theory Using a Coherent State Formulation," (Proceedings of Symposia on Density Matrices and Density Functionals in honor of A.J. Coleman); Reidel 1986, Eds. R.M. Erdahl and V.H. Smith.
88. B. Weiner and Y. Öhrn, "Correlated Electronic States of the LiH Molecule Studied with the Polarization Propagator," *J. Phys. Chem.* **91**, 563 (1987).
89. E. Deumens, B. Weiner, and Y. Öhrn, "Time-Dependent Variational Principle on the Group $SO(2r)$; Generalizations of Time-Dependent Hartree-Fock" *Nuclear Physics* **A466**, 85 (1987).
90. E. Sangfelt, R. Roychowdhury, B. Weiner, Y. Öhrn, "Generalized Tamm-Dancoff Approximation (GTDA) and Random-Phase Approximation (GRPA) Calculations on LiH, Be, and Li_2 ," *J. Chem. Phys.* **86**, 4523 (1987).

91. L. Lathouwers, P. Van Leuven, E. Deumens, and Y. Öhrn, "Applications of the Generator Coordinate Approximation to Diatomic Systems: II Dunham Analysis of Vibration-Rotation Spectra," *J. Chem. Phys.* **86**, 6352 (1987).
92. E. Deumens, L. Lathouwers, and Y. Öhrn, "A Dynamical Approach to Electron Transfer Reactions," *Int. J. Quantum Chem.* **S21**, 321 (1987).
93. E. Deumens and Y. Öhrn, "Electron-Nuclear Dynamics with Diabatic and Adiabatic Wave Packets," *J. Phys. Chem.* **92**, 3181 (1988).
94. E. Deumens and Y. Öhrn, "Time-Dependent Dynamics Applied to Electron Transfer" in, *Resonances* **325**, Eds. E. Brändas and N. Elander, (Springer Verlag, Berlin 1989) p. 233.
95. E. Deumens and Y. Öhrn, "Time-Dependent Dynamics of a Determinantal State," *Journal of Molecular Structure*, THEOCHEM **199**, 23 (1989).
96. C.R. Sarma, J. Paldus and Y. Öhrn, "Spin-Adaptation of Antisymmetrized Geminal Product Wavefunctions," *Int. J. Quantum Chem.* **36**, 35 (1989).
97. Y. Öhrn, "Propagator Methods for Molecular Electronic *Lecture Notes in Chemistry* Vol. **50** (Springer Verlag, New York 1989) Ed. D. Mukherjee.
98. J. Linderberg, Y. Öhrn, B. Vessal, S. Padkjaer, "Numerical Implementation of Reactive Scattering Theory," *J. Chem. Phys.* **90**, 6254 (1989).
99. J. Linderberg, Y. Öhrn, S. Padkjaer, "Gaussian-like Quadrature Rules for Quantum Mechanical Calculations," *J. Chem. Phys.* **91**, 4793 (1989).
100. E. Deumens and Y. Öhrn, "General Harmonic Approximation for Time-Dependent Molecular Dynamics", *Int. J. Quantum Chem.* **S23**, 31 (1989).

101. A. Diz, E. Deumens, and Y. Öhrn, "Quantum Electron-Nuclear Dynamics", *Chem. Phys. Lett.* **166**, 203 (1990).
102. J. Broeckhove, M. Claessens, L. Lathouwers, P. Van Leuven, E. Deumens, and Y. Öhrn, "Applications of the Generator Coordinate Approximation to Diatomic Systems. III. Curve-Crossing Problems", *J. Chem. Phys.* **93**, 8945 (1990).
103. B. Weiner, E. Deumens, and Y. Öhrn, "Coherent State Formulation of Multi-Configuration States" *J. Math. Phys.***32**, 1166 (1991).
104. B. Weiner, E. Deumens, and Y. Öhrn, "Spin Projection of Fermion Coherent States", *J. Math. Phys.* **32**, 2413 (1991).
105. L. Eriksson, Y. Öhrn, and G. Bergson, "Semiempirical MO-Study of Charge Transfer in (4-Aminophenyl)borane and Related Compounds-Molecular "Paddle-Wheels" " *Journal of Molecular Structure THEOCHEM*, **257**, 325 (1992).
106. J. Linderberg and Y. Öhrn, "Isoparametric Finite Elements on Hyperspheres", in *Advances in Molecular Vibrations and Collision Dynamics: Reactive Scattering*, Vol. IIA, p 33-45, edited by J. M. Bowman, JAI, Greenwich, Connecticut 1993.
107. E. Deumens, A. Diz, H. Taylor, and Y. Öhrn, "Time-Dependent Dynamics of Electrons and Nuclei", *J. Chem. Phys.* **96**, 6820 (1992).
108. Y. Öhrn, E. Deumens, A. Diz, R. Longo, J. Oreiro, and H. Taylor, "Time Evolution of Electrons and Nuclei in Molecular Systems", in *NATO ASI Series B: Physics* Vol. **299**, p 279-292, Plenum Press Editors J. Broeckhove and L. Lathouwers, 1992.
109. Y. Öhrn and O. Goscinski, "Analysis of the Thouless coherent state using the $1/K$ expansion", *Phys. Rev.* **A48**, 1093 (1993).
110. R. Longo, E. Deumens, and Y. Öhrn, " H^+ , H, He, H_2 scattering using a new time-dependent method for electron nuclear dynamics", *J. Chem. Phys.* **99**, 4554 (1993).

111. Y. Öhrn and E. Deumens, "Electron Nuclear Dynamics with Coherent States" in the *Proceedings of the International Symposium on Coherent States: Past, Present, and Future* held at Oak Ridge Associated Universities, June 14-17, 1993, p407-419, World Scientific, New Jersey 1994, Editors: D. H. Feng, J. R. Klauder, and M. R. Strayer.
112. B. Weiner, E. Deumens, and Y. Öhrn, "Coherent State Approach to Electron Nuclear Dynamics with an Antisymmetrized Geminal Power State", *J. Math. Phys.* **35**, 1139, (1994).
113. B. Champagne and Y. Öhrn, "Ab Initio Longitudinal Polarizabilities of Conjugated Stereoregular Polymers with a Carbon Backbone", *Chem. Phys. Letters.* **217**, 551 (1994).
114. E. Deumens, A. Diz, R. Longo, and Y. Öhrn, "Time-dependent Theoretical Treatments of the Dynamics of Electrons and Nuclei in Molecular Systems", *Reviews of Modern Physics* **66**, 917-983 (1994).
115. R. Longo, A. Diz, E. Deumens, and Y. Öhrn, "Influence of Electronic-Nuclear Coupling on Dynamics" *Chem. Phys. Letters* **220**, 305 (1994).
116. J.-L. Calais, E. Deumens, and Y. Öhrn, "A Model for Electron Nuclear Dynamics of a Monatomic Chain" *J. Chem. Phys.* **101**, 3989 (1994).
117. R. Longo, B. Champagne, and Y. Öhrn, "Electron Propagator Theory and Application", *Theoretica Chimica Acta* **90**, 397 (1995).
118. A. Diz and Y. Öhrn, "Electron-Nuclear Dynamics of Molecular Systems", *Int. J. Quantum Chem.* **S28**, 11 (1994).
119. J. Morales, A. Diz, E. Deumens, and Y. Öhrn, "Molecular Vibrational State Distributions in Collisions" *Chem. Phys. Lett.* **233**, 392 (1995).
120. A. Diz, Y. Öhrn, and J. R. Sabin, "Dynamic Charge States and Energy Deposition of Swift Helium Ions in Neon." *Nucl. Instr. Meth.* **B96**, 633 (1995).
121. J. Morales, A. Diz, E. Deumens, and Y. Öhrn, "Electron nuclear dynamics of $H^+ + H_2$ collisions at $E_{cm} = 20$ eV.", *J. Chem. Phys.* **103**, 9968 (1995).

122. Y. Öhrn, J. Oreiro, and E. Deumens, "Bond making and bond breaking in molecular dynamics", *Int. J. Quantum Chem.* **58**, 583 (1996); (Proceedings from the symposium The Chemical Bond held in honor of Jens Peder Dahl, July, 1994 at H. C. Ørsted Institute, Copenhagen, Denmark.)
123. B. Champagne, J.-M. André, and Y. Öhrn, "Ab initio Dynamic Polarizabilities of Polymers. I. Hydrogen Chain Models." *Int. J. Quantum Chem.* **57**, 811 (1996).
124. B. Champagne, D. H. Mosley, J. G. Fripiat, J. M. André, and Y. Öhrn, "Comment on 'Size Consistency and Size Extensivity of Linear Response Properties using the Perturbed Electron Propagator'" [*J. Chem. Phys.* 102, 8967(1995)], *J. Chem. Phys.* **104**, 1166 (1996).
125. G. Bergson, J.-L. Calais, J. Morales, and Y. Öhrn, "Vibrational Motion in Isotopomers of the HeH⁺ Molecular Ion; An Application of the Electron Nuclear Dynamics Method", *Int. J. Quantum Chem.* **63**, 415 (1997).
126. E. Deumens and Y. Öhrn, "Phase Space Approach to the Dynamics of Molecular Systems", *J. Chem. Soc., Faraday Trans.* **93**, 919 (1997).
127. D. Jacqemin, J. A. Morales, E. Deumens, and Y. Öhrn, "Electron nuclear dynamics of proton collisions with methane at 30 eV." *J. Chem. Phys.* **107**, 6146 (1997).
128. B. Champagne, E. Deumens, and Y. Öhrn, "Vibrations and soliton dynamics of positively charged polyacetylene chains" *J. Chem. Phys.* **107**, 5433 (1997).
129. J. Broeckhove, M. D. Coutinho-Neto, E. Deumens, and Y. Öhrn, "The electron nuclear dynamics of LiH and HF in an intense laser field", *Phys. Rev. A* **56**, 4996 (1997).
130. M. Hedström, J. A. Morales, E. Deumens, and Y. Öhrn, "Electron nuclear dynamics of H⁺ + H₂O collisions" *Chem. Phys. Lett.* **279**, 241 (1997).

131. M. Hedström, E. Deumens, and Y. Öhrn, "Electron nuclear dynamics of charge transfer collisions of protons with atomic oxygen." *Phys. Rev. A* **57**, 2625 (1998).
132. R. Cabrera-Trujillo, J. R. Sabin, Y. Öhrn, and J. Oddershede, "Oscillator strength sum rules with an external electromagnetic field", *Phys. Rev. A* **57**, 3115 (1998).
133. J. A. Morales, E. Deumens, and Y. Öhrn, "On rotational coherent states in molecular quantum dynamics", *J. Math. Phys.* **40**, 766 (1999).
134. M. Coutinho Neto, E. Deumens, and Y. Öhrn, "Selective Bond Breaking in the H + HOD Reaction", *Int. J. Quantum Chem.* **77**, 301 (2000).
135. Y. Öhrn and E. Deumens, "Towards an *ab initio* treatment of the time-dependent Schrödinger equation of molecular systems", *J. Phys. Chem. A* **103**, 9545 (1999).
136. R. Cabrera-Trujillo, J. R. Sabin, Y. Öhrn, and E. Deumens, "Direct differential cross section calculations for ion-atom, and atom-atom collisions in the keV range." *Phys. Rev. A* **61**, 032719(1-7) (2000).
137. R. Cabrera-Trujillo, E. Deumens, Y. Öhrn, and J. R. Sabin, "Impact parameter dependence of electronic and nuclear energy loss of swift ions: $H^+ \rightarrow He$ and $H^+ \rightarrow H$ ", *Nucl. Instr. Meth* **B168** 484-492 (2000).
138. R. Cabrera-Trujillo, J. R. Sabin, Y. Öhrn, and E. Deumens, "Charge Exchange and Threshold Effects in the Energy Loss of Slow Projectiles", *Phys. Rev. Lett.* **84**, 5300 (2000).
139. R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, and J. R. Sabin, "Stopping cross section in the low- to intermediate energy range: Study of protons on atomic N, O, and F", *Phys. Rev. A* **62**, 052714(1-9) (2000).
140. R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn, "Stopping cross section and charge exchange study on the $He^+ \rightarrow Ne$ system, Application of reactors in research and industry: Sixteenth International Conference *AIP Conference Proceedings*, **562**, 3 (2000).

141. E. Deumens and Y. Öhrn, "Complete Electron Nuclear Dynamics". *J. Phys. Chem. A* **105**, 2660 (2001).
142. A. Blass, E. Deumens, and Y. Öhrn, "Rovibrational Analysis of Molecular Collisions using Coherent States" *J. Chem. Phys.* **115**, 8633 (2001).
143. R. Cabrera-Trujillo, Y. Öhrn, J. R. Sabin, and E. Deumens, "Molecular target and projectile angular scattering effects in stopping power and charge exchange at low to intermediate energies", *Phys. Rev. A* **65**, 024901 (2002).
144. R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, and J. R. Sabin, "Trajectory and molecular binding effects in stopping cross section for hydrogen beams on H₂" *J. Chem. Phys.* **116**, 2783 (2002).
145. M. Coutinho-Neto, E. Deumens, and Y. Öhrn, "Abstraction and Exchange Mechanisms for the D₂ + NH₃⁺ Reaction at Hyperthermal Collision Energies" *J. Chem. Phys.* **116**, 2794 (2002).
146. Y. Öhrn and E. Deumens, "Electron Nuclear Dynamics" in *Effects of Electronic Degenerate States on Nuclear Dynamics Processes* Adv. Chem. Phys. Vol. **124**, 323-353 (Eds. Michael Baer and Gerd D. Billing) Wiley& Sons, New York, 2002.
147. Y. Öhrn, "Density, Density Matrix, or Propgator", *Adv. Quantum Chem.* Vol. **41** p. 35 (2002) ,Ed. J. R. Sabin.
148. S. A. Malinovskaya, R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn, "Dynamics of collisions of protons with acetylene molecules at 30 eV." *J. Chem. Phys.* **117**, 1103 (2002).
149. R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn, "Stopping Cross Sections for N⁴⁺ → H at Low Projectile Velocity", *Phys. Rev. A* **66**, 022706-(1-7) (2002).
150. D. Jacquemin, B. Champagne, J-M. André , E. Deumens, and Y. Öhrn, "Integral algorithm and density matrix integration scheme for *ab initio* band structure calculations on polymeric systems" *J. Comp. Chem.*, **23**, 1430-1444 (2002).

151. R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, J. R. Sabin, and B. G. Lindsay, "Theoretical and experimental studies of the $H^+ + N_2$ system: Differential cross sections for direct and charge-transfer scattering at keV energies", *Phys. Rev. A* **66**, 042712 (2002).
152. R. Cabrera-Trujillo, J. R. Sabin, Y. Öhrn, and E. Deumens, "Energy loss studies of protons colliding with ethane: Preliminary results", *J. Elec. Spectr.* **129**, 303-308 (2003).
153. R. Cabrera-Trujillo, J. R. Sabin, Y. Öhrn, and E. Deumens, "Case for Projectile Kinetic Energy Gain in Stopping Power Studies", *Int. J. Quantum Chem.* **94**, 215-221 (2003).
154. R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn, "Calculations of cross sections in Electron Nuclear Dynamics" *Adv. Quantum Chem.* **47**, 251-272, (2004).
155. R. Cabrera-Trujillo, J. R. Sabin, and Y. Öhrn, "Dynamical Processes in Stopping Cross Sections", *Adv. Quantum Chem.* **45**, 99-124 (2004).
156. R. Cabrera-Trujillo, J. R. Sabin, Y. Öhrn, and E. Deumens, "Stopping of swift antiprotons by hydrogen atoms and the Barkas correction", *Phys. Rev. A*, **71**, 012901 (2005).
157. R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, and J. R. Sabin, "Application of END Theory to the $H + D_2 \rightarrow HD + D$ reaction." *J. Phys. Chem. A* **108**, 8935-8940 (2004).
158. R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, J. R. Sabin, and B. G. Lindsay "Absolute differential and total cross sections for direct and charge-transfer scattering of keV protons by O_2 " *Phys. Rev. A* **70**, 042705 (2004).
159. Yngve Öhrn, "Jan Linderberg, Scientist, Teacher, Friend" *Adv. Quantum Chem.* **50**, xii-xix, (2005).
160. Yngve Öhrn and Erik Deumens, "A Dynamical Time-Dependent View of Molecular Theory", p. 9-40 in *Theory and Applications of Computational Chemistry: The First 40 Years, A volume of Technical and Historical Perspectives* (Elsevier 2005) Editors: C. E. Dykstra, G. Frenking, K. S. Kim, and G. E. Scuseria.

161. R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn, "Prediction of the Energy Dependence of Molecular Fragmentation Cross Sections for Collisions of Swift Protons with Ethane and Acetylene" *Phys. Rev. A*. **71**, 044702, (2005).
162. B. Killian, R. Cabrera-Trujillo, E. Deumens, and Y. Öhrn, "Resonant charge transfer between H^+ and H from 1 to 5000 eV" *J. Phys. B: At, Mol, Opt. Phys.* **37**, 1-15 (2004).
163. R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn, "Orientational Effects in Energy Deposition by Protons in Water", *Adv. Quantum. Chem.***48**, 47-57 (2005).
164. D. Masiello, E. Deumens, and Y. Öhrn, "Dynamics of an atomic electron and its electromagnetic field in a cavity", *Phys. Rev. A*.**71** 032108, (2005).
165. D. Masiello, E. Deumens, and Y. Öhrn, "On the canonical formulation of electrodynamics and wave mechanics", *Adv. Quantum Chem.***49**, 249-297 (2005).
166. Y. Öhrn and E. Deumens, "Time-Dependent, Direct, Nonadiabatic, Molecular Reaction Dynamics" in *Quantum Dynamics of Complex Molecular Systems*, Springer Series in Chemical Physics Vol. 83, 2006 Eds. D. Micha and I. Burghart.
167. N. Stolterfoht, R. Hellhammer, Z. Pesic, R. Cabrera-Trujillo, E. Deumens, Y. Öhrn, and J. R. Sabin, "Charge exchange and fragmentation in slow collisions of He^{2+} with water molecules", *Adv. Quantum Chem.*, **52**, 149-170 (2007).
168. R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn, "Theoretical Investigation of Energy Deposition and Electron Capture Cross Sections for Helium Ion Impact on Formaldehyde", Proceedings from the CAARI Conference, *Nucl. Instr. Meth.* **261**, 118-120 (2007).
169. R. Cabrera-Trujillo, E. Deumens, Y. Öhrn, O. Quinet, J. R. Sabin, and N. Stolterfoht, "Water molecule fragmentation induced by charge exchange in slow collisions with He^+ and He^{2+} ions in the keV region", *Phys. Rev. A* , **75**, 052702(13) (2007). **Reprinted** in *Virtual Journal*

of *Ultrafast Science* Vol. 6, Issue 6, June 2007 published on line by APS and AIP.

170. N. Stolterfoht, R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, R. Hoekstra, and J. R. Sabin, “Strong isotope effects on the charge transfer in slow collisions of He^{2+} with atomic hydrogen, deuterium, and tritium” *Phys. Rev. Lett.* (accepted) (2007).
171. Y. Öhrn, “Time-Dependent Molecular Reaction Dynamics”, AIP Proceedings of the ICCMSE 2007 (to appear)
172. J. R. Sabin, R. Cabrera-Trujillo, L. T. Chadderton, Y. Öhrn, and E. Deumens, “ Directional Aspects of Swift Ion Stopping in a Proto-Biological Molecule: Formaldehyde”, AIP Proceedings of ICCMSE 2007 (to appear).
173. Y. Öhrn and E. Deumens, “Time scales in molecular reaction dynamics”, Proceedings of the Summer School in Multiscale Simulations and modeling, held at Bosön, Sweden, June, 2007, Vol. xxx, Springer Series in Science.

Books

- J. Linderberg and Y. Öhrn, ”Propagators in Quantum Chemistry.” (Academic Press, London, 1973) 151 pages
- Y. Öhrn, ”Elements of Molecular Symmetry”, (Wiley&Sons, New York, 2000)
- J. Linderberg and Y. Öhrn, ”Propagators in Quantum Chemistry, Second Edition”. 267 pages (Wiley, Interscience, New York, 2004)

Books Edited

- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory and Quantum Statistics, Supplement **S8** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1974) 517 pages.

- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory and Quantum Statistics, Supplement **S9** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1975) 583 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory and Quantum Statistics, Supplement **S10** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1976) 439 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, Collision Phenomena and Computational Methods, Supplement **S11** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1977) 656 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, Collision Phenomena and Computational Methods, Supplement **S12** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1978) 545 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, Collision Phenomena, Quantum Statistics and Computational Methods, Supplement **S13** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1979) 722 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, Collision Phenomena, Quantum Statistics and Computational Methods, Supplement **S14** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1980) 734 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, Collision Phenomena and Computational Quantum Chemistry, Supplement **S15** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1981) 730 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, Collision Phenomena and Computational Quantum Chemistry, Supplement **S16** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1982) 674 pages.

- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, and Computational Quantum Chemistry, Supplement **S17** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1983) 650 pages.
- "Methods and Structures of Quantum Science," Plenum Press (1976) 595 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, and Computational Quantum Chemistry, Supplement to International Journal of Quantum Chemistry **S18**, John Wiley and Sons, New York (1984) 750 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, Scattering Problems, Many-Body Phenomena, and Computational Quantum Chemistry, Supplement to International Journal of Quantum Chemistry **S19**, John Wiley and Sons, New York (1985) 750 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, Scattering Problems, and Computational Quantum Chemistry, International Journal of Quantum Chemistry **S20**, John Wiley and Sons, New York (1986) 788 pages.
- Proceedings of the International Symposium on Quantum Chemistry, Solid-State Theory, and Computational Methods, Supplement **S21** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1987) 768 pages.
- Proceedings of the International Symposium on Quantum Chemistry, Solid-State Theory, and Computational Methods, Supplement **S22** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1988) 744 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory, and Molecular Dynamics, Supplement **S23** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1989) 732 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Solid-State Physics, and Computational Methods, Supplement **S24** to

International Journal of Quantum Chemistry, John Wiley and Sons, New York (1990) 892 pages.

- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, and Computational Methods, Supplement **S25** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1991) 704 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, and Computational Methods, Supplement **S26** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1992) 894 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, and Computational Methods, Supplement **S27** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1993) 828 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, and Computational Methods, Supplement **S28** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1994) 712 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, and Computational Methods, Supplement **S29** to International Journal of Quantum Chemistry, John Wiley and Sons, New York (1995) 708 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, and Computational Methods, *International Journal of Quantum Chemistry*, **60**, No. 7 (**S30**) John Wiley and Sons, New York (1996) 512 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, and Computational Methods, *International Journal of Quantum Chemistry*, **65**, No. 5 (**S31**) John Wiley and Sons, New York (1997) 650 pages.
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, *International Journal of Quantum Chemistry*, **70**, No. 4/5, 529-1098, John Wiley and Sons, New York (1998).

- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, *International Journal of Quantum Chemistry*, **75**, No. 4/5, 327-965, John Wiley and Sons, New York (1999).
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, *International Journal of Quantum Chemistry*, **80**, No. 4/5, 507-1135, John Wiley and Sons, New York (2000).
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, *International Journal of Quantum Chemistry*, **85**, No. 4/5, 171-635, John Wiley and Sons, New York (2001).
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, *International Journal of Quantum Chemistry*, **90**, No. 4/5, 1265-1554, John Wiley and Sons, New York (2002).
- Proceedings of the International Symposium on Atomic, Molecular and Condensed Matter Theory, *International Journal of Quantum Chemistry*, **95**, No. 4/5, 345-657, John Wiley and Sons, New York (2003).
- Proceedings of the International Symposium on Theory and Computations in Molecular and Materials Sciences, Biology and Pharmacology, *International Journal of Quantum Chemistry*, **100**, No. 6, 833-1196, John Wiley and Sons, New York (2004).
- Proceedings of the International Symposium on Theory and Computations in Molecular and Materials Sciences, Biology and Pharmacology, *International Journal of Quantum Chemistry*, **105** No. 6, 534-945, John Wiley and Sons, New York (2005).
- Proceedings of the International Symposium on Theory and Computations in Molecular and Materials Sciences, Biology and Pharmacology, *International Journal of Quantum Chemistry*, **106** No. 15, 3001-3401, John Wiley and Sons, New York (2006).

Administration and Service

University Administration and Service

- Chairman, Committee to Oversee the Separation of the Department of Astronomy and Physics, University of Florida into Two Departments, September 1979.
- Chairman, University Committee to Review the Department of Botany, University of Florida, 1982.
- Chairman, Search and Screen College Committee for Associate Dean of Liberal Arts and Sciences, 1988.
- Chairman, Search and Screen Committee for Vice President for Research and Dean of Graduate School, 1992/93.
- Chairman of the Long Range Committee of the Chemistry Department 1983-87
- Chairman of numerous Search and Screen Committees for Chemistry and Physics Faculty.
- Member of University Personnel Board, 1984-85.
- Member of Dean's Advisory Council, College of Liberal Arts and Sciences, 1991-94.
- Member of Search and Screen committee for Administrative Vice President, 2000-01
- Member of the University of Florida Athletic Association Board of Directors, 2000-02
- Judge at Research Forum of the Soil and Water Science Department at UF, September 5, 2002.
- Member of University Taskforce to make recommendations on policy regarding graduate student tuition charges on grant proposals 2002.
- Chair of the UF Senate Nominating Committee. 2002.
- Member of University Search and Screen Committee for Provost 2004.
- Member of the committee of the University Center for Excellence in Teaching (UCET) to award University Master Teachers 2004-05

- Member of Committee to select UF Teacher/Scholar of 2005/2006.

Recent National Professional Service

- Program Review Panel for DOE Combustion Program, November, 1992.
- Proposal Review Panel for DOE Radiation and Chemical Physics Program, December 1992.

Recent International Professional Service

- Dissertation committee of Denis Jacquemin, at the Department of Chemistry, University of Namur, Belgium **1998**.
- Member of International Committee of the Francqui Foundation, Belgium to select the laureate of the Franqui Prize. Meeting at Bruxelles, April, **2000**.
- Member of the evaluation and selection committee of candidates for a faculty position in Quantum Chemistry at the University of Copenhagen, Denmark, June **2000**.
- Member of the evaluation and selection panel of candidates for a Swedish Research Council faculty position in Theoretical Dynamics in Chemistry, June **2000**

Graduated Students

- **Joseph E. Kouba**, B.S., IIT, Chicago, Illinois; Ph.D., 1970; Ph.D. Thesis: "Theoretical Studies of Atom-Atom Interactions," with Professor Öhrn; NSF-Fellow 1970-71, at Aarhus University, Aarhus, Denmark. Now Technology Advisor, Mobile Oil Corp., Fairfax, VA.
- **Jess L. Thompson**, B.S., Southern Illinois University; M.S., 1971; M.S. Thesis: "A Symmetry Adapted Configuration Interaction Calculation of the Lithium Molecule," with Professor Öhrn. Now at Columbus Air Force Base, Missouri.

- **Rodney J. Bartlett**, B.S., Millsaps College; Ph.D., 1971; Ph.D. Thesis: "The Reduced Partitioning Procedure in CI Studies," with Professor Öhrn. NSF-Fellow 1971-72, Aarhus University, Aarhus, Denmark. Currently Graduate Research Professor of Chemistry and Physics, University of Florida.
- **Nelson H.F. Beebe**, B.S., McGill University, Canada; Ph.D., 1972; Ph.D. Thesis: "General Spin-Orbitals for Three-Electron Systems," with Professor Öhrn. Research Professor of Mathematics, University of Utah, Salt-Lake City, UT.
- **Jack A. Smith**, B.S., Purdue University, Indiana, 1971; M.S., 1973; Ph.D., 1978. M.S. Thesis: "HF-MO-LCGTO-SCF Calculations on H_2O and H_2O^+ ;" Ph.D. Thesis: "A Projected Hamiltonian Approach to Polyatomic Systems," with Professor Öhrn. Postdoctoral Position at the University of Florida, 1978-79. Scientist with Union Carbide, South Charleston, West Virginia.
- **George D. Purvis III**, B.S., Davidson College, N.D., 1969; Ph.D., 1973; Ph.D. Thesis: "Calculation of the Electron Propagator for Atoms and Molecules," with Professor Öhrn. VP CaChe Systems, Beaverton, Oregon.
- **R. Lynn Tyner-Redmon**, B.A. (Music) University of Florida, 1970; M.S. (Engineering) University of Florida, 1973; Ph.D. (Chemical Physics) University of Florida, 1975, with Professor Öhrn. Research Scientist at Batelle Institute, Columbus, Ohio.
- **Henry A. Kurtz**, B.S. Georgia Tech, Georgia, 1972, Ph.D. 1977; Ph.D. (Chemical Physics) Thesis: "Calculation of Electron Binding Energies," with Professor Öhrn. Professor of Chemistry and Dean of Science, University of Memphis, Tennessee.
- **Gregory Born**, B.S. Southern Illinois University, 1973, Ph.D., 1979; Ph.D. (Chemical Physics) Thesis: "Alternative Decouplings of the Electron Propagator," with Professor Öhrn. Research Scientist, RAND Corporation, Santa Monica, CA.
- **Manoj K. Mishra**, B.S. Ranchi University, India, 1971, Ph.D., 1981; Ph.D. (Chemical Physics) Thesis: "A Correlated Treatment of Bound

Continuum Transition within the Electron Propagator Formalism,” with Professor Öhrn. Professor of Chemistry, India Institute of Technology, Bombay, India.

- **Vincent Ortiz**, B.S., University of Florida, 1976, Ph.D., 1981; Ph.D. (Chemical Physics) Thesis: ”Propagator Calculations on Molecular Ionization and Excitation Processes” with Professor Öhrn. Chair and Ruth W. Mowlette Professor of Chemistry and Biochemistry at Auburn University, Alabama.
- **Rina Basu Roychowdhury**, B.S., University of Calcutta, Ph.D. 1985; Ph.D. (Chemical Physics) Thesis: ”Polarization Propagator Calculations for Open and Closed Shell Systems,” with Professor Öhrn. Assist. Prof. Department of Chemistry, American River College, 4700 College Oak Dr. Sacramento, CA 95841.
- **Agustín Carlos Diz** Licenciatura en Ciencias Físicas, University of Buenos Aires, Argentina, 1985; Ph.D. (Physics) 1992 Thesis: ”Electron-Nuclear Dynamics: A Theoretical Treatment Using Coherent States and the Time-Dependent Variational Principle” with Professor Öhrn. VP with SPF Oil Company, Barcelona, Spain.
- **Ricardo Luiz Longo** M. S. Chemistry, Federal University of Pernambuco, Brazil, 1988. Ph.D. (Chemistry) 1993 Thesis: ”Exploring a New Time-Dependent Method for Molecular Quantum Dynamics” with Professor Öhrn. Professor of Chemistry, the Federal University of Pernambuco, Recife, Brazil.
- **Benny Mogensen** B. S. in Chemistry from Copenhagen University, Denmark, 1992. Ph. D. (Quantum Chemistry) at Copenhagen University, 1997, Thesis: ”A Novel Approach to Electron Molecule Reactions”, with Professor Öhrn. Software engineer with Nokia Mobile Phones, Copenhagen, Denmark.
- **Juan Oreiro** M. S. degree in chemistry from the Federal University of Rio de Janeiro 1988. Ph. D. (Chemistry) 1997 Thesis: ”Analysis of the H_2^+ with H_2 Reaction Using Electron Nuclear Dynamics”. with Professor Öhrn. President of his own company in Brazil/Spain.

- **Jorge A. Morales** M. S. degree in chemistry from the National University of Mar del Plata, Argentina, 1989. Ph. D. (Chemistry) 1997 Thesis "Quasi-Classical and Semiclassical Formulation of the Electron Nuclear Dynamics Theory: A Method for Molecular Dynamical Processes". with Professor Öhrn. Associate Professor of Chemistry, Texas Tech University, Lubbock, TX.
- **Magnus Hedström** B.S. in physics from Uppsala University, Sweden. Ph. D. (Quantum Chemistry) at Uppsala University, Sweden, 1997, Thesis: "A Time-Dependent Approach to Adiabatic and Non-Adiabatic Molecular Dynamics Using Generalized Coherent States". with Professor Öhrn. Scientist at the Danish Technical University, Copenhagen, Denmark.
- **Ted A. O'Brien**, Ph. D. Student of the late Professor Michael C. Zerner, finished his dissertation in 2000 with Professor Öhrn.
- **Xuehe Zheng** Student of the late Professor Michael C. Zerner, finished his dissertation in 2000 with Professor Öhrn.
- **Mauricio Coutinho Neto**, Ph. D. (Chemistry) University of Florida, 2001. Dissertation: "Application of the Electron Nuclear Dynamics Theory to Hydrogen Abstraction and Exchange Reactions of $H + HOD$ and $D_2 + NH_3^+$ ". Assistant Professor at University of ABS (San Andre, SanBernardo, San Caetano), Brazil.
- **Anatol Blass**, Ph. D. (Physics) University of Florida, 2001. Dissertation: "Quasiclassical and Semiclassical Methods in Molecular Scattering Dynamics". Scientist with IBM.
- **David Masiello**, Ph.D. (Chemistry) University of Florida, 2004. Dissertation: "The Canonical Formulation of Electrodynamics and Wave Mechanics". Postdoctoral Associate at University of Washington, Seattle WA and at Northwestern University, Evanston, Illinois.
- **Benjamin J. Killian**, Ph. D. (Chemistry) University of Florida, 2005, Dissertation: "On Electronic Representations in Molecular Reaction Dynamics". Postdoctoral Associate, University of Maryland.

Postdoctoral Associates

Over thirty-five postdoctoral associates since 1967. They have gone on to successful careers in academe, government, and industry in U.S.A., Europe, Israel, and Japan.

Teaching

- General Chemistry, Physical Chemistry, Quantum Mechanics, Statistical Mechanics.
- Special topics: Molecular Reaction Dynamics.
- Special topics: Propagator Theory and Applications.

Special Projects

- Director of the annual International Sanibel Symposia on Quantum Chemistry and Solid-State Physics, organized by the Quantum Theory Project of the University of Florida (1983-2000)
- Co-Principal Investigator on special grants awarded for this activity: Office of Naval Research; National Science Foundation; Air Force Office of Scientific Research; Army Office of Scientific Research; Department of Energy; various computer hardware and software companies (1966-2000).
- Co-Principal Investigator on special cooperation grant from NATO to work with Aarhus University, Denmark, 1976-78, 1986-87, University of Antwerp, Belgium 1992-94.
- Co-Principal Investigator on a NATO grant sponsoring the Advanced Research Workshop on "Time-dependent Quantum Molecular Dynamics, Experiment and Theory", held at Snowbird, Utah, March 1992.
- Co-organizer of a one-week Short Course in Applied Molecular Orbital Theory offered 1988-1994 to about thirty participants, primarily from industry.

- Co-organizer of a workshop on Time-Dependent Quantum Molecular Dynamics, Brian Head, Utah, March 1999 funded by ONR.
- Organizer of Workshop on “Prospects for Theory, Computation, and Simulation in the Molecular Sciences in the 21’st Century”, at Spieterstulen, Norway, August 2-7, 2006.

References

- Professor John R. Sabin, Department of Physics, University of Florida, Gainesville, Florida 32611, sabin@qtp.ufl.edu
- Professor Jan Linderberg, Aarhus University, Aarhus C, DK 8000, DENMARK, jan@chem.au.dk
- Professor Mark Ratner, Department of Chemistry, Northwestern University, Evanston, Illinois 60201
- Professor Jean-Marie André, FUNDP, Namur, BELGIUM
- Professor J. Vincent Ortiz, Auburn University, Auburn, Alabama.
- Professor John P. Simons, Department of Chemistry, University of Utah, Salt Lake City, Utah 84112 simons@chem.utah.edu