

Physical and Chemical Properties Division
National Institute of Standards and Technology
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Education

Ph.D. in Chemistry California Institute of Technology, Pasadena, California Thesis: <i>Gas-Phase Chemistry of Organotransition Metal Ions</i> Advisor: Prof. J. L. Beauchamp	June 1991
A.B. in Chemistry (<i>summa cum laude</i>) Harvard College, Cambridge, Massachusetts	June 1984

Awards

Sigma Xi Young Scientist Award (NIST chapter) (1998)
National Research Council Research Associateship (6/91-6/93)
National Science Foundation Predoctoral Fellowship (9/84-9/87)

Experience

Government Research

Conducted *ab initio* calculations to identify and solve problems in thermochemistry, chemical kinetics, molecular spectroscopy, and peptide ion fragmentation. Developed new computational techniques for reaction prediction, reaction energetics and molecular spectroscopy. Developed “virtual measurements” methods for obtaining uncertainties associated with predictions from quantum chemistry. (National Institute of Standards and Technology, 6/93-present)

Postdoctoral Research

Conducted exploratory studies and characterization of free radicals and other reactive intermediates using resonance-enhanced multiphoton ionization spectroscopy. Employed *ab initio* calculations to clarify and extend the spectroscopic measurements. (J. W. Hudgens, National Institute of Standards and Technology, 7/91-6/93)

Used advanced *ab initio* quantum chemical techniques to study the structure and energetics of reactive organometallic and bio-organic species. (W. A. Goddard III, California Institute of Technology, 1/91-6/91)

Graduate Research

Studied numerous transition-metal ions using both experimental and theoretical techniques. Employed Fourier-transform mass spectrometry to study thermochemistry and reactivity of organometallic, inorganic, and bio-inorganic ions in the gas phase. Discovered gas-phase methane oligomerization chemistry. Addressed questions in interstellar chemistry and physical organic chemistry using quantum and classical theoretical methods. (J. L. Beauchamp, California Institute of Technology, 9/84-12/90)

Undergraduate Research

Conducted molecular dynamics calculations on B- and Z-DNA oligomers. (M. Karplus, Harvard, 2/83-6/84)

Synthesized substituted acridines. (S. A. Benner, Harvard, 2/82-6/82)

Industrial Research

Investigated kinetics of olefin hydroformylation catalyzed by soluble rhodium complexes. (A. A. Oswald, Exxon Research and Engineering Co., Summer 1983)

Studied alkane dehydrocyclization and aromatization over zeolite-supported platinum catalysts. (S. J. Tauster, Exxon Research and Engineering Co., Summer 1982)

Teaching

Designed and delivered lectures and laboratory course on *ab initio* thermochemistry (NATO ASI, Castelo Branco, Portugal, 7/98)

Designed and taught course on *ab initio* methods in chemical kinetics and thermodynamics (National Institute of Standards and Technology, 5/96-6/96)

Teaching assistant for graduate biophysical chemistry (two years) and for freshman chemistry (three years). Duties included grading, classroom teaching, demonstrations, and composition of problem sets and examinations. (California Institute of Technology, 9/84-6/89)

Grading for general chemistry and laboratory preparation for organic chemistry course with 350 students. (Harvard, 9/83-6/84)

Technical Skills

Ab Initio Software: GAUSSIAN (J. A. Pople *et al.*), GAMESS-US (M. S. Gordon *et al.*), ACES II (R. J. Bartlett *et al.*), MOLPRO (H.-J. Werner and P. J. Knowles), MOLCAS (B. O. Roos *et al.*), MOLFDIR (W. C. Nieuwpoort *et al.*), MOLECULE-SWEDEN (J. Almlöf *et al.*), MQM (W. A. Goddard III *et al.*), COLUMBUS (R. Shepard *et al.*)

Computers: Experience with Perl, awk, C, HTML, Fortran, Basic, PHP/MySQL, Pascal, Java, assembler

Resonance-Enhanced Multiphoton Ionization Spectroscopy

Fourier-Transform Ion Cyclotron Resonance Spectrometry (FTMS)

Lasers: Excimer, dye, Nd:YAG, CO₂

Vacuum Technology: Ultrahigh vacuum methods and equipment, pulsed valves, TOF-MS.

Foreign Languages: Written and spoken French (intermediate) and German (weaker)

Professional Service

Secretary, NIST chapter of Sigma Xi, 2003-2005.

Organizer, symposium on "Connections between Theory and Experiment," 16th IUPAC Conference on Chemical Thermodynamics, Halifax, Nova Scotia, Canada, August 6-11, 2000.

Organizing committee, NATO Advanced Study Institute, "Energetics of Stable Molecules and Reactive Intermediates," Castelo Branco, Portugal, July 14 - 24, 1998.

Organizer, symposium on "Computational Thermochemistry," 212th ACS National Meeting, Orlando, Florida, August 25-29, 1996.

Refereeing for journals and granting agencies (most frequently for *J. Phys. Chem.*, *Int. J. Mass. Spectrom.*, and *J. Am. Chem. Soc.*)

Professional Memberships

American Chemical Society ([ACS](#))

American Physical Society ([APS](#))

American Society for Mass Spectrometry ([ASMS](#))

Sigma Xi, The Scientific Research Society ([ΣΞ](#))

Publications (~60 journal papers and book chapters) [link](#)

Technical Presentations (~25 invited and ~50 contributed presentations) [link](#)