

Personal Data:

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Educational Background:

Ph. D. Biophysics, December, 1979, University of California, Davis, CA
B. A. Physics, June, 1971, California Lutheran College, Thousand Oaks, CA

Fields of specialization: Computational chemistry and physical biochemistry, the structure and function of metalloproteins, and structural bioinformatics.

Professional Experience:

7/94- Professor of Chemistry & Biochemistry, Middlebury College:
6/04-6/05 Visiting Professor of Medicinal Chemistry, University of Utah, Salt Lake City, Utah
6/93-9/93 Research Associate at the Research Institute of Scripps Clinic, Molecular Biology:
12/88-6/93 Associate Professor of Chemistry & Biochemistry, Middlebury College:
6/87-9/87 Research Associate at the Research Institute of Scripps Clinic, Molecular Biology:
9/84-11/88 Assistant Professor of Chemistry, Middlebury College:
9/83-9/84 Visiting Assistant Professor, Middlebury College:
9/82-9/83 Visiting Assistant Professor, Univ. of California, Davis:
9/81-9/82 Lecturer, California State Univ. Sacramento:
1/80-9/81 Postdoctoral researcher, Univ. of California, Davis:
9/78-12/79 Graduate Student, Univ. of California, Davis:
9/76-9/78 Lecturer, Illinois State University:
9/71-6/76 Graduate Student, Univ. of California, Davis:

Courses Taught at Middlebury**Chemistry and Biochemistry courses**

CH 103 Fundamentals of Chemistry I (Lecture and laboratory)
CH 104 Fundamentals of Chemistry II (Lecture and Laboratory)
CH 107 Advanced General Chemistry (Lecture and Laboratory)
CH 311 Instrumental Analysis Laboratory (Lecture and Laboratory)
CH 312 Inorganic and Physical Chemistry (Laboratory)
CH 324 Structural Bioinformatics (Lecture and Laboratory)
CH 351 Microscopic Physical Chemistry (Lecture and Discussion)
CH 352 Physical Chemistry of Macromolecules (lecture and discussion)
CH 353 Physical Biochemistry (Lecture and Discussion)
CH 400 Seminar in Chemical Research
CH 431 Advanced Inorganic Chemistry (Lecture and Discussion)
CH 452 Special Topics in Physical Chemistry: NMR (lecture and Laboratory)
CH 500 Independent Research Project
CH 700 Senior Research and Thesis

Winter Term

ID 23.2 The Ascent of Man: A New Chapter

CH 241	Organic Chemistry I (Laboratory)
ID 22.9	Microcomputer Interfacing for the Non-Scientist
CH 33.7	Molecular Modeling Laboratory
CH 39	Chemical Applications of Group Theory
ID 014	What Is Life (Lecture and Laboratory)
CH 314	Bioinformatics (Lecture and Laboratory)

First year writing intensive seminars

FS 025	What is Life?: Schrödinger, Crick, Dyson and Snow
FS 008	The Ascent of Man: "Science and Human Values"
FS 052	What is Life (Lecture and Laboratory)

Grants:

- 2005 "Molecular Dynamic Studies of the Vibrational A States of Carboxy-myoglobin", NSF-PACI 50,000 computer hours. Funded
- 2003 "Development of Force Fields for the Knowledge-based Prediction of Protein Folding", Vermont-VGN, \$10,000
- 1995 "Molecular Mechanics Laboratory for Undergraduate Instruction", NSF-ILI-IP \$41,961,
- 1992 "NSF summer NMR workshop at Rensselaer Polytechnic Institute", NSF \$1000
- 1991 "Electronic Structures of Catalase and Related Proteins", NIH \$98,007
- 1988 "Spin Coupling in Biologically Important Porphyrin π -Cation Radicals" VT-EPSCoR \$3917
- 1985 "A Cooperative Multidepartmental Computer facility for Undergraduate Science Laboratories", NSF , \$30,766
- 1985 "Theoretical Analysis of Enzymatic Low Valence Iron Oxo Complexes", Research Corporation \$12,000.
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Student Research Projects:

- 2006 Thesis: "Molecular Dynamic Studies of the Electrostatic Effects on the Vibration of Heme Bound Ligands in Myoglobin", Jakub Kostal
- 2005 Summer research: "Molecular Dynamic Studies of the Vibrational A States of Carboxy-myoglobin", Jakub Kostal
- 2005 Summer research: "Characterization of Penicillin Binding Proteins in *Borrelia burgdorferi*", Meghan Beucher
- 2005 Thesis: "Protein Homology Models of Putative Carboxypeptidases in *Borrelia burgdorferi*" Amrita Sarkar
- 2004 Thesis: "Homology Models of Putative Carboxy-Peptidases in *Borrelia burgdorferi*" James Reed Gahagan

- 2004 Independent Study: "Folding of Penicillin Binding proteins" Amrita Sarkar
- 2003 Summer research: "Protein Homology Models of Putative Carboxypeptidases in *Borrelia burgdorferi*" Amrita Sarkar
- 2001 Independent study: "The Large Ribosomal Subunit: a structure/function tutorial" Zack Lesko
- 2001 Independent study: "Force Field for protoporphyrin IX" Amanda Hakemian
- 2000 Summer research: "Normal Mode Analysis of Heme Ligands" Liqin Lu
- 2000 Thesis: "Modeling of CO bound to Heme and Myoglobin" Sohail Yousufi
- 2000 Thesis: "Molecular Dynamic Simulations of the A-states of Carboxy Myoglobin," Derek D. Prabharasuth
- 1998 Thesis: "Normal Mode Analysis of Carbonmonoxy-Myoglobin and Related Small Molecules," Ivan I. Beraha
- 1997 Summer Research: "Normal Mode Analysis of Carbonmonoxy-Myoglobin and Related Small Molecules," Ivan I. Beraha
- 1997 Thesis: "Vibration Analysis of Heme Porphyrin" Vikram Sundar
- 1996 Summer research: "Vibration Analysis of Heme Porphyrin" Vikram Sundar
- 1996 Thesis: "Parameterization of a Transferable Force Field for Nickel Octaethyl Porphyrin," Jason W. Dimmig
- 1995 Summer Research: "Parameterization of a Transferable Force Field for Nickel Octaethyl Porphyrin," Jason W. Dimmig
- 1994 Thesis: "Molecular Dynamics of Carbon Monoxide Photodissociation from Myoglobin," Maggie Zraly
- 1994 Summer Research: "Molecular Dynamics of Carbon Monoxide Photodissociation from Myoglobin," Maggie Zraly
- 1993 Thesis: "Symmetry Analysis of C₆₀ Fullerene," Amy Kimball
- 1993 Independent study: "Synthesis and Spectroscopy of C₆₀ Fullerenes," Abel L. Rives
- 1991 Summer research project on computer aided instruction: Schrodinger's equation in one-dimension. Colin Tan and Matthew Benjamin
- 1990 Thesis: "Synthesis and NMR Analysis of Copper Tetraphenylporphyrin and its π -Cation Radical," Chris Daigle
- 1990 Independent study: "Experimental Studies on Metalloporphyrins and their Cation Radicals," Steve Hanna

- 1989 Summer student research project on NMR of Copper Porphyrins. Chris Daigle
- 1988 Summer student research project on spin coupling in porphyrin cation radicals. Steve Hanna
- 1987 Thesis: "The Structure and Function of the Active Oxygen Intermediate of Cytochrome P-450," Thomas Cheatham.
- 1986 Summer student research project on Cytochrome P-450 and computer graphics. Thomas Cheatham and Yonik Seely
- 1985 Summer student research project on Cytochrome P-450 and peroxidase. Thomas Mellow and Matthew Benz.
- 1984 Thesis: "Feasibility of the use of P-31 NMR in the study of Pyridoxal-5'-phosphate - Steroid Hormone Receptor Interaction", David Sherris.

Professional Activities:

Member of the American Chemical Society	1972 - present
Chairman, Chemistry Department, Middlebury College	1987,1989-92,1994-97
Program Director of Molecular Biology and Biochemistry	2005 - present
Outside Referee for Faculty Reviews: Clarmont McKenna College	1998
Campus Ombudsperson	1994-97
Paper review, The Chemical Educator	1995-present
Bicentennial Hall Building Committee	1995-1999
NIH grant review panel	1995
Premedical Committee member, Middlebury College	1984-87,1999,2000,2003-04
Honorary Degree Committee, Middlebury College	2001-02
Junior/Senior faculty relations Committee, Middlebury College	1989-90
Independent Scholars Committee, Middlebury College	1989-90
Athletic Policy committee, Middlebury College	1991-93
Computer committee, Middlebury College	1988,1992
Paper review, Journals of the American Chemical Society	1988-90
Book review, Richard Wolfson's undergraduate Physics Text.	1988

Work in progress:

My current research deals with the development and applications of structural bioinformatics methods to the problem of predicting the three-dimensional folded structure of proteins. The concerted effort during this last decade to sequence genomes has resulted in over ten million new protein sequences but only thirty thousand protein crystal structures have been determined. Accurate prediction of protein structure from sequence data would open up the vast genome sequence information to direct inquiry about the biological function of genes. We have been focusing on structural predictions for ten genes found in *Borrelia burgdorferi*, the Lyme disease bacteria, which are thought to have a role in antibiotic resistance to penicillin. Lyme disease is the most common vector-borne disease in the United States with over 22,000 cases recorded in 2002. We are addressing this protein folding problem using both bioinformatics and experimental molecular biology methods. It is exciting to see how the recent explosion of information contained in nucleic acid and protein databases has opened a broad new class of methods for predicting protein structure. Research talks about this work can be found on our web site

<http://cat.middlebury.edu/~chem/>

Presentations:

* Indicates student co-authors

- 2005 Byers, J. H.; Zhang, Y.*; Zegarelli, B.M.*; Dimitrova, T.*; Huque, S.*; Sontum, S. F. "Radical Reactions mediated by Cyclobutadieneiron Tricarbonyl" Presented at National Organic Symposium, Salt Lake City UT, 6/12/05. Abstract A38.
- 2003 "Protein Homology Models of Putative Carboxypeptidases in *Borrelia burgdorferi*", with Amrita Sarkar*, Second Mercury Conference, August 2003, Hamilton College
- 1999 "Graphical 3-D Animation in the Normal Mode Analysis of Small Molecules", with Ivan I. Beraha*, Chemistry & the Internet - ChemInt'99: September 25, 1999 Washington DC.
- 1999 "Normal Mode Analysis of Heme within Myoglobin and Related Small Molecules", with Ivan I. Beraha*, Jason W. Dimmig*, and Vikram C. Sundar*, National American Chemical Society meeting: March 21, 1999 Anaheim California
- 1998 "Normal Mode Analysis of Carbonmonoxy-Myoglobin and Related Small Molecules", with Ivan I. Beraha*, National American Chemical Society meeting: August 24, 1998 Boston Massachusetts
- 1998 "Normal Mode Analysis of Carbonmonoxy-Myoglobin and Related Small Molecules", with Ivan I. Beraha*, Eastern New York Section of the American Chemical Society undergraduate Chemistry Research Symposium: April 18, 1998 Skidmore College
- 1995 "Functional Protein Cavities Molecular Dynamics of Carbon Monoxide within Myoglobin", with M. A. Zrally* and M. W. Roberson
National American Chemical Society meeting: April 5, 1995 Anaheim California

- 1994 "Molecular Dynamics of the Metastable B-State of Carbon Monoxide after Photodissociation from Myoglobin", with M. A. Zrally*, S. P. Mitchell*, and M. W. Roberson, 24th American Chemical Society North East Regional Meeting
University of Vermont, Burlington, VT
- 1991 "A Macintosh Program for Quantum Chemistry in One Dimension" with S.J. Chisdes*, T. Mahmud*, M. Benjamin*, and C. Tan*
21th American Chemical Society North East Regional Meeting
University of Massachusetts, Amherst, MA
- 1990 "Spin Coupling in Porphyrin π -Cation Radicals" with C.C. Daigle* and S.D. Hanna*
Fourth National Conference on Undergraduate Research
Union College, Schenectady, New York
- 1988 "d-Orbital Spin Coupling in Metalloporphyrin π -Cation Radicals" with D. A. Case, T. E. Cheatham*
American Chemical Society National Meeting
Toronto, Canada
- 1987 "Axial Ligand Effects on the Electronic Structure of Fe(IV) Porphyrin Complexes" with Thomas Cheatham* and Thomas Mellow*
17th A.C.S. North East Regional Meeting
Rochester, N.Y.
- 1985 "Theoretical Analysis of Enzymatic Low-Valent Iron Oxo Complexes" with Matt Benz* and Thomas Mellow*
5th International Congress on Quantum Chemistry
Montreal, Canada.
- 1984 "A Theoretical Analysis of Fe(IV) Active Site Models for Compound I and II of Peroxidase" with D.A. Case
American Chemical Society National Meeting
Philadelphia, PA.
- 1983 "X-alpha Multiple Scattering Calculations on Fe(IV) Active Site Models of Compound I and II of Peroxidase" with D.A. Case
Fifth West Coast Theoretical Chemistry Conference
Stanford Research Institute, Palo Alto, CA.
- 1981 "A Theoretical Analysis of the Ground and Excited States of Deoxyhemoglobin" with D.A. Case
Third West Coast Theoretical Chemistry Conference
NASA Ames Research Center, Moffett Field, CA.
- 1980 "The Calculation of Isoelectronic Energy Differences Using Perturbation Series Expansions" with W.H. Fink and L.L. Ingraham
Second West Coast Theoretical Chemistry Conference,
California Institute of Technology, Pasadena, CA.

Invited presentations:

- 1988 "The Relationship Between Choosing a Wife and Choosing Research"
Middlebury College
- 1986 "Color and the Physical Chemistry of Heme:
What Every Red Blooded American Should Know."
Middlebury College
- 1983 "Single crystal Polarized Spectroscopy of Hemoglobin"
Middlebury College
- 1983 "Oxygen Activation in Peroxidase and Catalase"
Middlebury College
- 1983 "Spectroscopy of Biologically Important Metalloporphyrins"
Eastern Michigan University
- 1982 "Symmetry and the Spectroscopy of Hemes"
University of North Carolina, Wilmington
- 1981 "Theoretical and Spectroscopic Probes of Hemoglobin's
Structure and Function"
California State University at Sacramento

Published Papers:

- 2006 "Radical Reactions mediated by Cyclobutadieneiron Tricarbonyl"; Byers, J. H., Sontum S.F., Zhang, Y.*; Zegarelli, B.M.*; Dimitrova, T.*; Huque, S.*, Jasinski, J.*. Butcher, R.*. Organometallics June 2006
- 1989 "Electronic Structure in Broken-Symmetry and Spin-Symmetry: Applications to Fe-S Proteins and Clusters"; L. Noodleman, D.A. Case, S. F. Sontum; Journal De Chime Physique et De Physicochime Biologique 86:743, 1989
- 1989 "A Laser Refraction Method for Measuring Liquid Diffusion Coefficients"; Robert Pitha, Mackenzie King and Stephen Sontum; Journal of Chemical Education 66:787, 1989
- 1989 "Spin Coupling and Electron Delocalization in Mixed Valence Iron Sulfur Clusters"; S.F. Sontum, L. Noodleman and D.A. Case; American Chemical Society Symposium Series **394**; "Computational Chemistry: The Challenge of d and f Electrons" D.R. Salahub and M.C. Zerner eds; pp 366-377, 1989.
- 1985 "Electronic Structures of Active site Models for compounds I and II of Peroxidase."; Stephen Sontum and David Case; Journal of the American Chemical Society, 107:4013, 1985.
- 1983 "Xalpha multiple scattering calculations on Iron(II) porphine."; Stephen Sontum, David Case, and Martin Karplus; Journal of Chemical Physics 79:2881, 1983

- 1982 "Xalpha multiple scattering calculations on Copper, Silver and Gold porphines."; Stephen Sontum and David Case;
Journal of Physical Chemistry 86:1596, 1982
- 1981 "Calculations of isoelectronic energy differences using perturbation theory."; Stephen Sontum, Lloyd Ingraham, and William Fink;
International Journal of Quantum Chemistry 21:179, 1981
- 1979 "Photosolvolyis of 3,4-dichloroaniline in water: evidence for an aryl cation intermediate."; Glenn Miller, Michael Mille, Donald Crosby, Stephen Sontum, and Richard Zepp;
Tetrahedron 35:1797, 1979
- 1977 "Electronacceptor properties of chlorinated dibenzo-p-dioxins."; Donald Crosby, Glenn Miller, and Stephen Sontum.
Bulletin of Environmental Contamination and Toxicology 18:611, 1977
- 1977 "Computer simulation of the determination of amino acid sequence in polypeptides."; Stephen Daubert, and Stephen Sontum;
Journal of Chemical Education 54:35, 1977.
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Software: all software can be found on <http://cat.middlebury.edu/~chem/>

- 2006 "Structural Bioinformatics" Spring Course Web page:
<http://cat.middlebury.edu/~chem/chemistry/class/bio/ch324/>
- 2003 "Bioinformatics"; Winter Term Bioinformatics Course
Departmental Web page: <http://cat.middlebury.edu/~chem/class/bio/ch314>
- 2003 "parm_heme.dat" AMBER protein force field modified to include heme active sites.
Departmental Web page: <http://cat.middlebury.edu/~chem/software/heme/>
- 2002 "Normal Modes of Methylene Dichloride", a Java script/Chime tutorial on the normal modes of motion. Departmental Web page:
<http://cat.middlebury.edu/~chem/ch2cl2/vib.html>
- 2001 "The Large Ribosomal Subunit: a structure/function tutorial"; with Zack Lesko*, A Java script/Chime tutorial on the mechanism for protein translation
Departmental Web page:
<http://cat.middlebury.edu/~chem/class/physical/quantum/quantum.html>
- 1999 "Quantum"; with Sarah Chisdes*, Matthew Benjamin*, Colin Tan* and Matthew Sontum; A Java Applet to Solve Schrödinger's Equation in One-Dimension
Departmental Web page:
<http://cat.middlebury.edu/~chem/class/physical/quantum/quantum.html>
- 1998 "Hydrogen Atom"; A General Chemistry Laboratory Exercise and Tutorial on the Hydrogen Atom spectrum
Departmental Web page: <http://cat.middlebury.edu/~chem/class/general/ch103>
- 1998 "Lysozyme"; with Ryan David*, and Bob Cluss; A Biochemistry Laboratory Exercise and Tutorial on Enzyme Kinetics
Departmental Web page: <http://cat.middlebury.edu/~chem/class/bio/ch322>

- 1997 "Molecular Modeling"; Winter Term Molecular Modeling Course
Departmental Web page: <http://cat.middlebury.edu/~chem/students/wintermstu.html>
- 1994 "QuantumCalc"; Matthew Benjamin*, Colin Tan* and Stephen Sontum, a Quick Basic program to solve Shroedinger's equation in one dimension
Departmental Web page: <http://cat.middlebury.edu/~chem/software>
- 1994 "Xasw3"; David A. Case, Michael Cook, and Stephen Sontum, a FORTRAN program to do scattered wave quantum calculations
Departmental Web page: <http://cat.middlebury.edu/~chem/software>
- 1994 "CrystalCalc", Stephen Sontum, a Quick Basic program to demonstrate crystal structures
Departmental Web page: <http://cat.middlebury.edu/~chem/software>
- 1994 "ChemLedger", Stephen Sontum, a Quick Basic program to keep departmental ledgers
Departmental Web page: <http://cat.middlebury.edu/~chem/software>