

# Curriculum Vitae

## Stephen F. Sontum

### Personal Data:

Stephen F. Sontum  
Department of Chemistry & Biochemistry  
Middlebury College  
Middlebury, VT. 05753

Married, Two children  
Office phone: (802)443-5445  
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Internet: sontum@middlebury.edu

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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 bioinformatics.

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### Professional Experience:

7/94- Professor of Chemistry & Biochemistry, Middlebury College:

Taught first year general chemistry, physical chemistry, advanced laboratory, organic laboratory, advanced inorganic chemistry, bioinformatics, and first year seminar courses. Principal investigator of a grant on Molecular Modeling in the undergraduate curriculum. Development of educational software for teaching. Reviewer for the Chemical Educator. Member of a NIH area grant review panel. Chairman of the department of chemistry and biochemistry for 1994-97. Program Director of the Molecular Biology and Biochemistry program 2005-

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: Leave year. Research on the molecular dynamics of DNA. Principal investigator of a NIH grant for studies on catalase. Developed research and teaching software.

12/88-6/93 Associate Professor of Chemistry & Biochemistry, Middlebury College:

Taught freshman chemistry, physical chemistry, advanced laboratory, organic laboratory, and freshman seminar courses. Principal investigator of grants for studies on peroxidase and catalase. Development of educational software for teaching. Chairman of the department of chemistry for 1989-92.

6/87-9/87 Research Associate at the Research Institute of Scripps Clinic, Molecular Biology: Leave year. Research on porphyrin spin states and the conversion of the XASW program from the VAX VMS to the SUN UNIX operating systems.

9/84-11/88 Assistant Professor of Chemistry, Middlebury College:

Taught freshman chemistry, physical chemistry and advanced laboratory courses. Supervision of thesis research in theoretical chemistry. Principal investigator of grant that established Science Center laboratory computers. Chairman of the department of chemistry for 1987.

9/83-9/84 Visiting Assistant Professor, Middlebury College:

Taught undergraduate freshman and physical chemistry courses. Supervision of thesis research in nuclear magnetic resonance.

9/82-9/83 Visiting Assistant Professor, Univ. of California, Davis:

Taught courses in physical chemistry lecture and laboratory, quantitative analysis and freshman inorganic chemistry. Supervised undergraduate research projects on NMR and oxaporphyrins.

9/81-9/82 Lecturer, California State Univ. Sacramento:

Taught a graduate course in physical chemistry and undergraduate courses in freshman chemistry. Research on hyperfine interaction problems in peroxidase.

1/80-9/81 Postdoctoral researcher, Univ. of California, Davis:

Laboratory coordinator for freshman chemistry courses. Research with Dr. Case on spin density distributions in metalloporphyrins.

9/78-12/79 Graduate Student, Univ. of California, Davis:

Thesis title: "Perturbation Theory Analysis of Iron(II) and Porphine Formation." A new perturbation theory was developed to study the enzymatic formation of heme.

9/76-9/78 Lecturer, Illinois State University:

Taught undergraduate courses in freshman chemistry and biochemistry. Taught graduate courses in physical biochemistry and chemical kinetics. Supervised undergraduate research projects on the ferrochelatase reaction.

9/71-6/76 Graduate Student, Univ. of California, Davis:

Teaching assistant for biochemistry lecture and laboratory. Voted outstanding departmental teaching assistant in 1974.

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### Courses Taught 1988-2006:

#### 1988 - 1989

Fall	CH 103	Fundamentals of Chemistry I (Lecture)
Fall	CH 351	Physical Chemistry I
Winter	ID 22.9	Microcomputer Interfacing for the Non-Scientist
Spring	CH 104L	Fundamentals of Chemistry II (Laboratory)
Spring	CH 312/311	Advanced Chemistry Laboratory I & II

#### 1989 - 1990

Fall	FS 025	Freshman Seminar: What is Life?
Fall	CH 311/312	Advanced Chemistry Laboratory I & II
Fall	CH 700	Senior Research and Thesis
Winter	CH 700	Senior Research and Thesis
Spring	CH 352	Physical Chemistry II
Spring	CH 104	Fundamentals of Chemistry II (Lecture)
Spring	CH 500	Independent Study Project
Spring	CH 700	Senior Research and Thesis

#### 1990 - 1991

Fall	CH 104	Fundamentals of Chemistry II (Lecture)
Fall	CH 351	Physical Chemistry I
Winter	CH 39	Chemical Applications of Group Theory
Spring	CH 353	Physical Chemistry for the Life Sciences
Spring	CH 104L	Fundamentals of Chemistry II (Laboratory)

**1991 - 1992**

Fall	CH 351	Physical Chemistry I (Lecture and Discussion)
Fall	CH 452	Physical Chemistry III
Winter	ID 23.2	The Ascent of Man: A New Chapter
Spring	CH 352	Physical Chemistry II (Lecture and Discussion)
Spring	CH 353	Physical Chemistry for the Life Sciences (Lecture and Discussion)

**1992 - 1993**

Fall	CH 103	Fundamentals of Chemistry I (Lecture)
Fall	CH 400	Seminar in Chemical Research
Fall	CH 700	Senior Research and Thesis
Fall	CH 104L	Fundamentals of Chemistry II (Laboratory)
Winter	CH 241	Organic Chemistry I (Laboratory)
Winter	CH 700	Senior Research and Thesis
Spring	CH 352	Physical Chemistry II (Lecture and Discussion)
Spring	CH 353	Physical Chemistry for the Life Sciences (Lecture and Discussion)

**1993 - 1994**

On Leave Academic Year 1993 - 1994

**1994 - 1995**

Fall	CH 103	Fundamentals of Chemistry I (Lecture)
Fall	CH 351	Physical Chemistry I (Lecture and Discussion)
Fall	CH 104L	Fundamentals of Chemistry II (Laboratory)
Fall	CH 700	Senior Research and Thesis
Winter	CH 700	Senior Research and Thesis
Spring	CH 103L	Fundamentals of Chemistry I (Laboratory)
Spring	CH 352	Physical Chemistry II (Lecture and Discussion)

**1995 - 1996**

Fall	FS008	The Ascent of Man: "Science and Human Values"
Fall	CH 452	Special Topics in Physical Chemistry: NMR (lecture and Laboratory)
Fall	CH 700	Senior Research and Thesis
Winter	CH 241	Organic Chemistry I (Laboratory)
Winter	CH 700	Senior Research and Thesis
Spring	CH 312	Advanced Chemistry laboratory II
Spring	CH 353	Physical Chemistry for the Life Sciences (Lecture and Discussion)
Spring	CH 700	Senior Research and Thesis

**1996 - 1997**

Fall	CH 104	Fundamentals of Chemistry II (Lecture)
Fall	CH 352	Physical Chemistry of Macromolecules (Lecture and Discussion)
Fall	CH 700	Senior Research and Thesis
Winter	CH 33.7	Molecular Modeling Laboratory
Winter	CH 700	Senior Research and Thesis
Spring	CH 104	Fundamentals of Chemistry II (Lecture)
Spring	CH 104	Fundamentals of Chemistry II (PreLab)
Spring	CH 104	Fundamentals of Chemistry II (Lab)
Fall	CH 700	Senior Research and Thesis

**1997 - 1998**

Fall	CH 103	Fundamentals of Chemistry I (Lecture)
Fall	CH 103	Fundamentals of Chemistry I (PreLab)
Fall	CH 352	Physical Chemistry of Macromolecules (lecture and discussion)
Fall	CH 700	Senior Research and Thesis
Winter	CH 700	Senior Research and Thesis
Spring	CH 103	Fundamentals of Chemistry I (Lecture)
Spring	CH 103	Fundamentals of Chemistry I (PreLab)
Spring	CH 353	Physical Chemistry for the Life Sciences (Lecture and Discussion)
Spring	CH 700	Senior Research and Thesis

**1998 - 1999**

On Leave Academic Year 1998 - 1999

**1999 - 2000**

Fall	CH 351	Microscopic Physical Chemistry (Lecture and Discussion)
Fall	CH 431	Advanced Inorganic Chemistry (Lecture and Discussion)
Fall	CH 700	Senior Research and Thesis
Winter	CH 700	Senior Research and Thesis
Spring	CH 104	Fundamentals of Chemistry II (Lecture)
Spring	CH 104	Fundamentals of Chemistry II (Laboratory)
Spring	CH 353	Physical Chemistry for the Life Sciences (Lecture and Discussion)
Spring	CH 700	Senior Research and Thesis

**2000 - 2001**

Fall	CH 103	Fundamentals of Chemistry I (Lecture)
Fall	CH 104/7L	Fundamentals of Chemistry II (Laboratory)
Fall	CH 431	Advanced Inorganic Chemistry (Lecture and Discussion)
Winter	ID 014	What Is Life (lecture and laboratory)
Spring	CH 312	Inorganic and Physical Chemistry Lab (Lecture and Discussion)
Spring	CH 353	Physical Biochemistry (Lecture and Discussion)
Spring	CH 500	Independent Research Project

**2001 - 2002**

Fall	CH 351	Microscopic Physical Chemistry (Lecture and Discussion)
Fall	CH 311	Instrumental Analysis Laboratory (Lecture and laboratory)
Fall	CH 500	Independent Research Project
Spring	FS 052	What is Life (Lecture and laboratory)
Spring	CH 353	Physical Biochemistry (Lecture and Discussion)

**2002 - 2003**

Fall	CH 311	Instrumental Analysis Laboratory (Lecture and laboratory)
Fall	CH 351	Microscopic Physical Chemistry (Lecture and Discussion)
Winter	CH 314	Bioinformatics (lecture and laboratory)
Spring	CH 352	Macroscopic Physical Chemistry (Lecture and Discussion))
Spring	CH 353	Physical Biochemistry (Lecture and Discussion)

**2003 - 2004**

Fall	CH 107	Advanced General Chemistry I (Lecture and Discussions)
Fall	CH 311	Instrumental Analysis Laboratory (Lecture and laboratory)
Fall	CH 700	Senior Research and Thesis
Winter	CH 700	Senior Research and Thesis
Winter	CH 500	Independent Research Project
Spring	CH 103	Fundamentals of Chemistry I (Lecture and Discussions)
Spring	CH 353	Physical Biochemistry (Lecture and Discussion)
Spring	CH 700	Senior Research and Thesis

**2004 - 2005**

On Leave Academic Year 2004 – 2005

Fall	CH 700	Senior Research and Thesis
Spring	CH 700	Senior Research and Thesis

**2005 - 2006**

Fall	CH 103	General Chemistry I (Lecture and Discussions)
Fall	CH 351	Microscopic Physical Chemistry (Lecture and Discussion)
Fall	CH 700	Senior Research and Thesis
Winter	CH 700	Senior Research and Thesis
Spring	CH 324	Structural Bioinformatics (Lecture and Laboratory)
Spring	CH 353	Physical Biochemistry (Lecture and Discussion)
Spring	CH 700	Senior Research and Thesis

**2006 - 2007**

Fall	CH 104	General Chemistry II (Lecture and Discussions)
Fall	CH 351	Microscopic Physical Chemistry (Lecture and Discussion)
Winter	CH 700	Senior Research and Thesis
Spring	CH 104	General Chemistry II (Lecture and Discussions)
Spring	CH 353	Physical Biochemistry (Lecture and Discussion)

**2007 - 2008**

Fall	CH 103	General Chemistry I (Lecture and Discussions)
Fall	CH 351	Microscopic Physical Chemistry (Lecture and Discussion)
Fall	CH 700	Senior Research and Thesis
Winter	CH 700	Senior Research and Thesis
Spring	CH 103	General Chemistry I (Lecture and Discussions)
Spring	CH 324	Structural Bioinformatics (Lecture and Laboratory)
Spring	CH 700	Senior Research and Thesis
Spring	MBBC700	Senior Research and Seminar

**2008 - 2009**

Fall	CH 351	Microscopic Physical Chemistry (Lecture and Discussion)
Fall	CH 700	Senior Research and Thesis
Fall	FS 1237	What is Life (Lecture and laboratory)
Winter	CH 700	Senior Research and Thesis
Spring	CH 353	Physical Biochemistry (Lecture and Discussion)
Spring	CH 324	Structural Bioinformatics (Lecture and Laboratory)
Spring	CH 700	Senior Research and Thesis
Spring	MBBC700	Senior Research and Seminar

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**Grant Applications:**

- 2008 Development of a New Binding Selective Homology Modeling Method for Proteins  
Vt EPSCOR \$15,000 pending
- 2007 Binding Selective Homology Models of Penicillin Binding Proteins in B.Burgdorferi,  
VGN \$64,963, Not funded
- 2006 Binding Selective Homology Models of Penicillin Binding Proteins in B.Burgdorferi,  
VGN \$24,591, Not funded
- 2005 "Molecular Dynamic Studies of the Vibrational A States of Carboxy-myoglobin", NSF-  
PACI 50,000 computer hours. Funded
- 2005 Characterization of Penicillin Binding Proteins in B. burgdorferi VGN \$150,000, Not  
funded
- 2004 "Folding of Penicillin Binding Proteins in B. burgdorferi", NIH-AREA \$203,248, Not  
funded
- 2003 "Design and Application of Force Fields for the Knowledge-based Prediction of Protein  
structure", PRF-UHF, \$50,000 not funded
- 2003 "Development of Force Fields for the Knowledge-based Prediction of Protein Folding",  
Vermont-VGN, \$10,000 funded
- 1998 "Development of a Force Field for Protein Bound Heme", NIH-AREA, \$75,000, not  
funded
- 1998 "Development of a Consistent Force Field for Protein Bound Heme" NSF-RUI  
\$154,961, not funded
- 1995 "Molecular Mechanics Laboratory for Undergraduate Instruction", NSF-ILI-IP \$41,961,  
funded.
- 1994 "Recombination Pathways in Myoglobin Mutants", NSF-CRUIP \$699,975,  
not funded.
- 1992 "NSF summer NMR workshop at Rensselaer Polytechnic Institute", NSF \$1000,  
funded.
- 1991 "Electronic Structures of Catalase and Related Proteins", NIH \$98,007, funded.
- 1989 "Electronic Structures of Catalase and Related Proteins", NIH \$105,026, approved  
with score 179, not funded
- 1988 "Spin Coupling in Biologically Important Porphyrin  $\pi$ -Cation Radicals"  
VT-EPSCoR \$3917, funded
- 1987 "Relativistic Analysis of the Ground and Excited States of Deoxyhemoglobin" VT-  
EPSCoR, \$3,660, not funded

- 1985 "A Cooperative Multidepartmental Computer facility for Undergraduate Science Laboratories", NSF , \$30,766, funded
- 1985 "Theoretical Analysis of Enzymatic Low Valence Iron Oxo Complexes", Research Corporation \$12,000, funded
- 1984 "Multi-disciplinary Science Laboratory Computers", NSF \$55,104, not funded
- 1981 NIH Postdoctoral Fellowship approved but none funded that year.
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**Student Research Projects:**

- 2008 Thesis:"Effects of mutations upon the vibrational A-states of carboxy-myoglobin", Nick Barone
- 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 Buecher
- 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 C<sub>60</sub> Fullerene," Amy Kimball
- 1993 Independent study: "Synthesis and Spectroscopy of C<sub>60</sub> 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  $\pi$ -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.

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**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



Faculty Reader Middlebury Admissions	2008-present
Outside Referee for Faculty Reviews: Claremont McKenna College	1998
Campus Ombudsperson	1994-97
Paper review, The Chemical Educator	1995-2004
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 the human genome has resulted in over ten million new gene sequences, which have no corresponding three-dimensional structural information. Accurate prediction of protein structure from sequence data would open up the vast GenBank data set 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, that 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. We presented our initial homology models for one of these genes this summer at the Mercury conference on computational chemistry. The results of our work can be found at our web site <http://www.middlebury.edu/~sontum/>

**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  $\pi$ -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  $\pi$ -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.
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**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
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**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* 25:3787, 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 Miille, 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://www.middlebury.edu/~sontum/>

- 2006 "Structural Bioinformatics" Spring Course Web page:  
<http://www.middlebury.edu/~sontum/chemistry/class/bio/ch324/>

- 2003 "parm\_heme.dat" AMBER protein force field modified to include heme active sites.  
Departmental Web page:  
<http://www.middlebury.edu/~sontum/chemistry/software/heme/>
- 2002 "Normal Modes of Methylene Dichloride", a Java script/Chime tutorial on the normal modes of motion. Departmental Web page:  
<http://www.middlebury.edu/~sontum/chemistry/ch2cl2/index.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://www.middlebury.edu/~sontum/chemistry/class/bio/ch322/ribosome/>
- 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://www.middlebury.edu/~sontum/chemistry/class/physical/quantum/quantum.html>
- 1998 "Hydrogen Atom"; A General Chemistry Laboratory Exercise and Tutorial on the Hydrogen Atom spectrum  
Departmental Web page:  
<http://www.middlebury.edu/~sontum/chemistry/class/general/ch103>
- 1998 "Lysozyme"; with Ryan David\*, and Bob Cluss; A Biochemistry Laboratory Exercise and Tutorial on Enzyme Kinetics  
Departmental Web page:  
<http://www.middlebury.edu/~sontum/chemistry/class/bio/ch322>
- 1997 "Molecular Modeling"; Winter Term Molecular Modeling Course  
Departmental Web page:  
<http://www.middlebury.edu/~sontum/chemistry/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://www.middlebury.edu/~sontum/chemistry/software>
- 1994 "Xasw3"; David A. Case, Michael Cook, and Stephen Sontum, a FORTRAN program to do scattered wave quantum calculations  
Departmental Web page:  
<http://www.middlebury.edu/~sontum/chemistry/software/ftp/unix/>
- 1994 "CrystalCalc", Stephen Sontum, a Quick Basic program to demonstrate crystal structures  
Departmental Web page:  
<http://www.middlebury.edu/~sontum/chemistry/software/ftp/mac/>
- 1994 "ChemLedger", Stephen Sontum, a Quick Basic program to keep departmental ledgers  
Departmental Web page:  
<http://www.middlebury.edu/~sontum/chemistry/software/ftp/mac/>