John E. STRAUB

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Boston University
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Boston, MA 02215

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Personal Data

Married with two children

Education

NIH Postdoctoral Fellow	Biophysics, Harvard University, 1987-1990 (with Martin Karplus$^{\otimes,\star}$)
Ph.D.	Chemical Physics, Columbia University, 1987 (with Bruce Berne$^{\otimes}$)
M. Phil.	Chemical Physics, Columbia University, 1986
M.A.	Chemical Physics, Columbia University, 1984
B.S.	Chemistry, University of Maryland, 1982 (with Millard Alexander)

Honors

United Methodist Church Scholar/Teacher of the Year, Boston University 2016

Japan Society for the Promotion of Science Invitation Fellow, Nagoya University, Nagoya, Japan 2014

J. T. Oden Faculty Fellow, University of Texas at Austin 2012

Henry Eyring Center Lecturer, University of Utah 2011

Phi Beta Kappa National Visiting Scholar 2011-2012

Metcalf Award for Excellence in Teaching, Boston University 2005

Gitner Award for Distinguished Teaching, Boston University 2003

Alfred P. Sloan Research Fellow 1995-1997

Pegram Research Award, Columbia University 1986

Graduate Teaching Award, Columbia University 1984

Employment History

2002-present	Professor of Chemistry
Spring 2014	Visiting Professor Department of Physics, Nagoya University, Nagoya, Japan
2006-2007	Visiting Professor Department of Chemistry and Biochemistry, Montana State University, Bozeman, Montana
1996-2002	Associate Professor of Chemistry Boston University, Boston, MA
Fall 1998	Visiting Professor Institute for Advanced Studies, Hebrew University (Givat Ram), Jerusalem, Israel
1990-1996	Assistant Professor of Chemistry Boston University, Boston, MA

Recent Professional Service (last 10 years)

The Journal of Chemical Physics, Associate Editor 2010-present

President, Telluride Science Research Center 2006-2008, 2016-present

Phi Beta Kappa Visiting Scholars Panel 2012-present

Board of Directors, Pinhead Institute 2009-2014

Biophysical Journal, Editorial Board Member 2006-2007

Selected University Service (last 5 years)

2012-2015	Co-Chair, Course Credit Definition Committee, Boston University
2014-2015	Appointment, Promotion and Tenure Committee, College of Arts and Sciences, Boston University
2007-2012	Chair, Department of Chemistry, Boston University

Workshop and Symposium Organization (last 5 years)

11-13 July 2016 CECAM Workshop on "Multiscale modeling of biomolecular aggregation and protein-membrane interactions in amyloid diseases," Lugano, Switzerland (co-organizer with Vio Buchete and Birgit Strodel)

15-20 December 2015 Symposium on "Conformational dynamics of biomolecules and the biomolecule-solvent interface," International Chemical Congress of Pacific Basin Societies "Pacifichem," Honolulu, Hawaii, (co-organizer with Masataka Nagaoka, David Leitner, and YiQin Gao)

22-26 March 2015 "Role of membrane in amyloid-formation and the pathogenicity of amyloid disease, American Chemical Society National Meeting, Denver, Colorado (co-organizer with Jennifer C. Lee)

19-23 May 2014 Workshop on "Protein dynamics," l'École de Physique des Houches, Les Houches, France (co-organizer with Martin Weik and Doug Tobias)

Research Supervision and Mentoring

Graduate Students (present)

George Pantelopulos$^{\bullet}$	2015-present	B.S. in Chemistry 2015
Asanga Bandara	2014-present	B.S. in Chemistry 2013

Postdoctoral Fellows (present)

Ryo Urano	2015-present	Ph.D. in Physics 2015
Afra Panahi$^{\diamond}$	2014-present	Ph.D. in Chemistry 2013

Postdoctoral Fellows (past)

Laura Dominguez$^{\odot}$	2012-2014	Ph.D. in Biochemistry Science 2011
Edyta Malolepsza	2009-2012	Ph.D. in Chemistry 2006
Adam Moser	2009-2012	Ph.D. in Chemistry 2009
Jaegil Kim	2007-2011	Ph.D. in Theoretical Physical Chemistry 2000
Susan DeSensi$^{\diamond}$	2007-2009	Ph.D. in Chemical and Physical Biology 2007
Christina Crecca$^{\diamond}$	2008-2009	Ph.D. in Chemistry 2008
Naoyuki Miyashita	2005-2007	Ph.D. in Functional Molecular Science 2003
Hiroshi Fujisaki	2003-2007	Ph.D. in Physics 2000
Alan van Giessen	2002-2005	Ph.D. in Chemistry 1999
Javier Guevara	1998-2000	Ph.D. in Physics 1998
Diane Sagnella^{+}	1998-2000	Ph.D. in Chemistry 1997

Graduate Students (past)

Qing Lu	2011-2015	Ph.D. in Materials Science and Engineering 2015
Leigh Foster	2008-2014	Ph.D. in Chemistry 2014
Anna Victoria Martinez	2008-2013	Ph.D. in Chemistry 2013
Ping Zhang	2007-2012	Ph.D. in Chemistry 2012
Eva Rivera	2002-2009	Ph.D. in Chemistry 2009
Yong Zhang	2003-2008	Ph.D. in Chemistry 2008
Bogdan Tarus	2001-2006	Ph.D. in Chemistry 2006
Lintao Bu	1999-2004	Ph.D. in Chemistry 2004
Nicolae-Viorel Buchete	1996-2003	Ph.D. in Chemistry 2003
Troy Whitfield	1996-2001	Ph.D. in Chemistry 2001
Francesca Massi	1995-2001	Ph.D. in Chemistry 2001
Shuanghong Huo	1994-1999	Ph.D. in Chemistry 1999

Ioan Andricioaei	1994-1999	Ph.D. in Chemistry 1999
Patricia Amara	1991-1996	Ph.D. in Chemistry 1996
Jianpeng Ma	1991-1995	Ph.D. in Chemistry 1996
Ji-Kyung Choi	1994-1995	M.A. in Chemistry 1995

Undergraduate Research Students

James Teruya (2016-present), Andrew Burwash (2016-present), Longjiaxin Zhong (2015-2016), Emily Schmidt (2014-2015), Paola Velez[†] (2013-2014), Derrick Lewis (2011-2013), Lani Rush (2010-2012), Will Ginsberg (2008-2009), Janice Ye (2007-2008), Edwin Landaker† (1994-1996), Sharon Motzkin (1994-1995), Ji-Kyung Choi[†] (1991-1994), Alissa Rashkin[†] (1990-1993), Deborah Pearlman (1990-1992)

High School Research Students

Eric Hu (2014), Dheekshita Kumar (2014), Zachary Ziegler (2011-2012), Nikhil Pradhan* (2004), Courtney Sargent* (2003), Arnold Oh* (2001), Shawn Anthony°#* (2000), Elizabeth Faist* (1999), Meagan Clement* (1997), Jonathan Chu* (1997), Brandy Evans* (1996), Daniel Sharfman* (1996), Eric Lo* (1995)

† Honors Thesis, Boston University, * Research Internship Program, Boston University, ◇ Postdoctoral Faculty Fellow, Boston University, ° Siemens-Westinghouse Science and Technology Competition Semifinalist, # Intel Science Talent Search Semifinalist, + NIH National Research Service Award, ⊙ Schlumberger Foundation Faculty for the Future, • NSF Graduate Research Fellowship, ⊗ National Academy of Sciences, ⋆ Nobel Prize in Chemistry 2013

Publications (last 10 years, h-index = 46 WoS or 54 Google Scholar)

Books

"Proteins: Energy, Heat and Signal Flow," D. M. Leitner and J. E. Straub, Editors, Taylor and Francis Group, CRC Press (Boca Raton, 2009).

Journal Articles

140. "Specific binding of cholesterol to C99 domain of Amyloid Precursor Protein depends critically on charge state of protein," A. Panahi, A. Bandara, G.A. Pantelopulos, L. Dominguez, and J.E. Straub, *J. Phys. Chem. Lett.* **7**, 3535-3541 (2016).

139. "Impact of membrane lipid composition on the structure and stability of the transmembrane domain of amyloid precursor protein," L. Dominguez, L. Foster, J.E. Straub, and D. Thirumalai, *Proc. Natl. Acad. Sci. USA* **113**, E5281-E5287 (2016).

138. "On the use of mass scaling for stable and efficient simulated tempering with molecular dynamics," T. Nagai, G.A. Pantelopulos, T. Takahashi, and J.E. Straub, *J. Comp. Chem.* **37**, 2017-2028 (2016).

137. "Combined molecular dynamics simulations and experimental studies of the structure and dynamics of poly-amido-saccharides," S.L. Chin, Q. Lu, E.L. Dane, L. Dominguez, C.J. McKnight, J.E. Straub, and M.W. Grinstaff, *J. Am. Chem. Soc.* **138**, 6532-6540 (2016).

136. "Freezing transitions of nanoconfined coarse-grained water show subtle dependence on confining environment," Q. Lu and J.E. Straub, *J. Phys. Chem. B* **120**, 2517-2525 (2016).

135. "Extension of a protein docking algorithm to membranes and applications to amyloid precursor protein dimerization," S. Viswanath, L. Dominguez, L. S. Foster, J. E. Straub, and R. Elber, *Proteins* **83**, 2170-2185 (2015).

134. "Role of charge and solvation in the structure and dynamics of alanine-rich peptide AKA_2 in AOT reverse micelles," A.V. Martinez, E. Malolepsza, L. Dominguez, Q. Lu, and J.E. Straub, *J. Phys. Chem. B* **119**, 9084-9090 (2015).

133. "Exploring the role of hydration and confinement in the aggregation of amyloidogenic peptides $A\beta_{16-22}$ and $Sup35_{7-13}$ in AOT reverse micelles," A.V. Martinez, E. Malolepsza, E. Rivera, Q. Lu, and J.E. Straub, *J. Chem. Phys.* **141**, 22D530 (2014).

132. "Investigating the solid-liquid phase transition of water nanofilms using the generalized replica exchange method," Q. Lu, J. Kim, J. D. Farrell, D. J. Wales, and J.E. Straub, *J. Chem. Phys.* **141**, 18C525 (2014).

131. "Empirical maps for the calculation of amide I vibrational spectra of proteins from classical molecular dynamics simulations," E. Malolepsza, and J.E. Straub, *J. Phys. Chem. B* **118**, 7848-7855 (2014).

130. "Propensity to form amyloid fibrils is encoded as excitations in the free energy landscape of monomeric proteins," P.I. Zhuravlev, G. Reddy, J.E. Straub, and D. Thirumalai, *J. Mol. Bio.* **426**, 2653-2666 (2014).

129. "Structural heterogeneity in transmembrane Amyloid Precursor Protein homodimer is a consequence of environmental selection," L. Dominguez, L. Foster, S.C. Meredith, J.E. Straub, and D. Thirumalai, *J. Am. Chem. Soc.* **136**, 9619-9626 (2014).

128. "Vibrational energy flow across heme-cytochrome c and cytochrome c-water interfaces," J. K. Agbo, Y. Xu, P. Zhang, J. E. Straub, and D. M. Leitner, *Theor. Chem. Acc.* **133**, 1504 (2014).

127. "Limit of metastability for liquid and vapor phases of water," W.J. Cho, J. Kim, J. Lee, T. Keyes, J. E. Straub and K.S. Kim, *Phys. Rev. Lett.* **112**, 157802 (2014).

126. "Membrane-protein interactions are key to understanding amyloid formation," J. E. Straub and D. Thirumalai, *J. Phys. Chem. Lett.* **5**, 633-635 (2014).

125. "Transmembrane fragment structures of Amyloid Precursor Protein depend on membrane surface curvature [Communication]," L. Dominguez, S.C. Meredith, J.E. Straub, and D. Thirumalai,*J. Am. Chem. Soc.* **136**, 854-857 (2014).

124. "Spatio-temporal hierarchy in the dynamics of a minimalist protein model," Y. Matsunaga, A. Baba, C.B. Li, J.E. Straub, M. Toda, T. Komatsuzaki, and R. S. Berry, *J. Chem. Phys.* **139**, 215101 (2013).

123. "'Strange Kinetics' in the temperature dependence of methionine ligand rebinding dynamics in cytochrome c," P. Zhang, S. W. Ahn, and J. E. Straub, *J. Phys. Chem. B* **117**, 7190-7202 (2013).

122. "Probing the structure and dynamics of confined water in AOT reverse micelles," A.V. Martinez, L. Dominguez, E. Malolepsza, A. Moser, Z. Ziegler, and J.E. Straub, *J. Phys. Chem. B* **117**, 7345-7351 (2013).

121. "Order parameter free enhanced sampling of the vapor-liquid transition using the generalized replica exchange method," Q. Lu, J. Kim, and J. E. Straub, *J. Chem. Phys.* **138**, 104119 (2013).

120. "Replica Exchange Statistical Temperature Molecular Dynamics algorithm," J. Kim, J. E. Straub, and T. Keyes, *J. Phys. Chem. B* **116**, 8646-8653 (2012).

119. "Exploring the solid-liquid phase change of an adapted Dzugutov model using Generalized Replica Exchange Method," Q. Lu, J. Kim, and J.E. Straub, *J. Phys. Chem. B* **116**, 8654-8661(2012).

118. "Dynamics of methionine ligand rebinding in cytochrome c," P. Zhang, E. Malolepsza, and J. E. Straub, *J. Phys. Chem. B* **116**, 6980-6990 (2012).

117. "Role of water in protein aggregation and amyloid polymorphism," D. Thirumalai, G. Reddy, and J. E. Straub, *Acc. Chem. Res.* **45**, 83-92 (2012).

116. "Non-Markovian theory of vibrational energy relaxation and its applications to bimolecular systems," H. Fujisaki, Y. Zhang, and J.E. Straub, *Adv. Chem. Phys.* **145**, 1-33 (2011).

115. "Ergodic problems for real complex systems in chemical physics," T. Komatsuzaki, A. Baba, M. Toda, J. E. Straub, and R. S. Berry, *Adv. Chem. Phys.* **45**, 171-220 (2011).

114. "Entropic stabilization of proteins by TMAO," S. S. Cho, G. Reddy, J.E. Straub, and D. Thirumalai, *J. Phys. Chem. B* **115**, 13401-13407 (2011).

113. "Communication: Iteration-free, weighted histogram analysis method in terms of intensive variables," J. Kim, T. Keyes, and J.E. Straub, *J. Chem. Phys.* **135**, 061103 (2011).

112. "Influence of nanoparticle size and shape on oligomer formation of an amyloidogenic peptide," E.P. O'Brien, J.E. Straub, B.R. Brooks, and D. Thirumalai, *J. Phys. Chem. Lett.* **2**, 1171-1177 (2011).

111. "Protein folding in a reverse micelle environment: The role of confinement and dehydration," A.V. Martinez, S.C. DeSensi, L. Dominguez, E. Rivera, and J.E. Straub, *J. Chem. Phys.* **134**, 055107 (2011).

110. "Toward a molecular theory of early and late events in monomer to amyloid fibril formation," J.E. Straub and D. Thirumalai, *Ann. Rev. Phys. Chem.* **62**, 437-463 (2011).

109. "Dry amyloid fibril assembly in a yeast prion peptide is mediated by long-lived structures containing water wires," G. Reddy, J.E. Straub, and D. Thirumalai, *Proc. Natl. Acad. Sci. USA* **107**, 21459-21464 (2010).

108. "Factors governing fibrillogenesis of polypeptide chains revealed by lattice models," M.S. Li, N.T. Co, G. Reddy, C.K. Hu, J.E. Straub, and D. Thirumalai, *Phys. Rev. Lett.* **105**, 218101 (2010).

107. "Generalized simulated tempering for exploring strong phase transitions," J. Kim and J.E. Straub, *J. Chem. Phys.* **133**, 154101 (2010).

106. "Generalized Replica Exchange Method," J. Kim, T. Keyes, and J.E. Straub, *J. Chem. Phys.* **132**, 224107 (2010).

105. "Principles governing oligomer formation in amyloidogenic peptides," J. E. Straub and D. Thirumalai, *Curr. Opin. Struc. Bio.* **20**, 187-195 (2010).

104. "Structures of β-amyloid peptide 1-40, 1-42, and 1-55-the 672-726 fragment of APP-in a membrane environment with implications for interactions with γ-secretase," N. Miyashita, J.E. Straub, and D. Thirumalai, *J. Am. Chem. Soc.* **131**, 17843-17852 (2009).

103. "Thermodynamic perspective on the dock-lock growth mechanism of amyloid fibrils," E.P. O'Brien, Y. Okamoto, J.E. Straub, B.R. Brooks and D. Thirumalai, *J. Phys. Chem. B* **113**, 14421-14430 (2009).

102. "Quantum and classical vibrational relaxation dynamics of N-methylacetamide on *ab initio* potential energy surfaces," H. Fujisaki, K. Yagi, J.E. Straub and G. Stock, *Int. J. Quant. Chem.* **109**, 2047-2057 (2009).

101. "Sequence and crowding effects in the aggregation of a 10-residue fragment derived from islet amyloid polypeptide," E. Rivera, J. [E.] Straub and D. Thirumalai, *Biophys. J.* **96**, 4552-4560 (2009).

100. "Direct evidence for mode-specific vibrational energy relaxation from quantum time-dependent perturbation theory. III. The ν_4 and ν_7 modes of nonplanar nickel porphyrin models," Y. Zhang and J.E. Straub, *J. Chem. Phys.* **130**, 215101 (2009).

99. "Optimal replica exchange method combined with Tsallis weight sampling," J. Kim and J.E. Straub, *J. Chem. Phys.* **130**, 144114 (2009).

98. "Transmembrane structures of amyloid precursor protein dimer predicted by Replica-Exchange Molecular Dynamics simulations," N. Miyashita, J.E. Straub, D. Thirumalai and Y. Sugita, *J. Am. Chem. Soc.* **131**, 3438 (2009).

97. "Dynamics of locking of peptides onto growing amyloid fibrils," G. Reddy, J. E. Straub, and D. Thirumalai, *Proc. Natl. Acad. Sci. USA* **106**, 11948-11953 (2009).

96. "Relationship between protein folding thermodynamics and the energy landscape," J. Kim and J.E. Straub, *Phys. Rev. E* **79**, 030902 (2009).

95. "Replica exchange statistical temperature Monte Carlo," J. Kim, T. Keyes and J.E. Straub, *J. Chem. Phys.* **130**, 124112 (2009).

94. "Mode-specific vibrational energy relaxation of amide I' and II' modes in N-methylacetamide/water clusters: Intra- and intermolecular energy transfer mechanisms," Y. Zhang, H. Fujisaki and J.E. Straub, *J. Phys. Chem. A* **113**, 3051-3060 (2009).

93. "Direct evidence for mode-specific vibrational energy relaxation from quantum time-dependent perturbation theory. II. The ν_4 and ν_7 modes of iron-protoporphyrin IX and iron porphine," Y. Zhang and J.E. Straub, *J. Chem. Phys.* **130**, 095102 (2009).

92. "Direct evidence for mode-specific vibrational energy relaxation from quantum time-dependent perturbation theory. I. Five-coordinate ferrous iron porphyrin model," Y. Zhang, H. Fujisaki and J.E. Straub, *J. Chem. Phys.* **130**, 025102 (2009).

91. "Influence of preformed Asp23-Lys28 salt bridge on the conformational fluctuations of monomers and dimers of Aβ peptides with implications for rates of fibril formation," G. Reddy, J. E. Straub and D. Thirumalai, *J. Phys. Chem. B* **113**, 1162-1172 (2009).

90. "Diversity of solvent dependent energy transfer pathways in heme proteins," Y. Zhang and J. E. Straub, *J. Phys. Chem. B* **113**, 825-830 (2009).

89. "Resilience of the iron environment in heme proteins," B.M. Leu, Y. Zhang, L.T. Bu, J. E. Straub, J.Y. Zhao, W. Sturhahn, E. E. Alp and J. T. Sage, *Biophys. J.* **95**, 5874-5899 (2008).

88. "Probing the mechanisms of fibril formation using lattice models," M. S. Li, D. K. Klimov, J.E. Straub and D. Thirumalai, *J. Chem. Phys.* **129**, 175101 (2008).

87. "Structures and free-energy landscapes of the wild type and mutants of the A beta(21-30) peptide are determined by an interplay between intrapeptide electrostatic and hydrophobic interactions," B. Tarus, J. E. Straub, and D. Thirumalai, *J. Mol. Bio.* **379**, 815-829 (2008).

86. "Dissecting contact potentials for proteins: Relative contributions of individual amino acids," N.-V. Buchete, J. E. Straub, D. Thirumalai, *Proteins* **70**, 119-130 (2008).

85. "Vibrational energy relaxation of isotopically labeled amide I modes in cytochrome c: Theoretical investigation of vibrational energy relaxation rates and pathways," H. Fujisaki and J.E. Straub, *J. Phys. Chem. B* **111**, 12017-12023 (2007).

84. "Structure optimization and folding mechanisms of off-lattice protein models using statistical temperature molecular dynamics simulation: Statistical temperature annealing," J. Kim, J.E. Straub and T. Keyes, *Phys. Rev. E* **76**, 011913 (2007).

83. "Quantum dynamics of N-methylacetamide studied by the vibrational configuration interaction method," H. Fujisaki, K. Yagi, K. Hirao, and J. E. Straub, *Chem. Phys. Lett.* **443**, 6-11 (2007).

82. "Statistical temperature molecular dynamics: Application to coarse-grained beta-barrel-forming protein models," J. Kim, J.E. Straub and T. Keyes, *J. Chem. Phys.* **126**, 135101 (2007).

81. "Molecular dynamics study on the solvent dependent heme cooling following ligand photolysis in carbonmonoxy myoglobin," Y. Zhang, H. Fujisaki, and J. E. Straub, *J. Phys. Chem. B* **111**, 3243-3250 (2007).

80. "Monomer adds to preformed structured oligomers of A β-peptides by a two-stage dock-lock mechanism," P.H. Phuong, M.S. Li, G. Stock, J.E. Straub, and D. Thirumalai, *Proc. Natl. Acad. Sci. USA* **104**, 111-116 (2007).

Book Chapters

B10. "On the development of coarse-grained protein models: Importance of relative side-chain orientations and backbone interactions," N.-V. Buchete, J. E. Straub and D. Thirumalai, in: *Coarse-Graining of Condensed Phase and Biomolecular Systems*, edited by G. A. Voth, Taylor & Francis Group/CRC Press (Boca Raton, Florida, 2009), pp. 141-156.

B9. "Scenarios for protein aggregation: Molecular Dynamics simulations and bioinformatics analysis," R. Dima, B. Tarus, G. Reddy, J. E. Straub and D. Thirumalai, in: *Protein Folding, Misfolding and Aggregation: Classical Themes and Novel Approaches*, edited by V. Muñoz, Royal Society of Chemistry Publishing (Cambridge, United Kingdom, 2008), pp. 241-265.

External Research Grant and Fellowship Support

Current and Anticipated External Support

1. NIH (R01 GM107703)
   "Probing the role of membrane and cholesterol on APP-C99 structure and dynamics"
   P.I. John E. Straub (co-PI Dave Thirumalai)
   3/1/15-2/28/19 ($1,183,824 total)
   For the development of a detailed understanding of the structure and dynamics of APP-C99 monomer and dimer, including the dependence on sequence and membrane environment.

2. NSF Chemistry Division (CHE-1362524)
   "Complex role of solvation in protein structure and dynamics in micelles and membranes"
   P.I. John E. Straub
   8/1/14-7/31/17 ($510,000 total)
   For the development of novel simulation approaches for the study of complex molecular systems involving membranes and micelles.

Past External Support (last 5 years)

21. NSF Chemistry Division (CHE-1114676)
   "Algorithms for the simulation of strong phase changes in complex molecular systems"
   P.I. John E. Straub
   6/15/11-5/31/14 ($500,000 total)
   For the development of novel simulation algorithms for the study of phase changes in molecular systems.

20. Schlumberger Foundation
   "Faculty for the Future Postdoctoral Fellowship"
   5/15/12-4/30/13 ($40,000 total)
   For the training of Dr. Laura Dominguez Duenas in the area of computational molecular biophysics.

19. NIH (R01 GM076688-08)
   "Probing the principles governing protein aggregation"
   P.I. John E. Straub
   12/15/05-11/30/11 ($1,543,375 total)
   For the theoretical and computational study of the principles of peptide and protein aggregation.

18. NSF Chemistry Division (CHE-0750309)
   "Probing the principles of dynamics and energy transfer in proteins"
   P.I. John E. Straub
   2/1/08-1/31/11 ($469,000 total)
   For the theoretical and computational study of the principles of energy transfer and signaling in proteins.

Teaching Experience and Science Outreach

Undergraduate Teaching Experience - Science for Non-Science Majors

CAS CC103 Core Natural Sciences II: The Evolution of Life and Intelligence
Undergraduate "Core" Curriculum, College of Arts and Sciences
F 1999

CAS CC106 Core Natural Sciences II: Biodiversity and the Evolution of Life
Undergraduate "Core" Curriculum, College of Arts and Sciences
S 2004, S 2005 (lecturer), S 2006 (lecturer)

Undergraduate Teaching Experience - Science for Science Majors

CAS CH101 General Chemistry
Undergraduate Course (1st semester)
S 1991, S 1992, F 1993, F 1995, F 1996, S 1999, F 2002, F 2003

CAS CH102 General Chemistry
Undergraduate Course (2nd semester)
S 1993, S 1994, S 1995, S 1996, S 2002, S 2003

CAS CH109 General and Quantitative Analytical Chemistry
Undergraduate Course (1st semester)
F 2015

CAS CH111 Intensive General and Quantitative Analytical Chemistry
Undergraduate Honors Course (1st semester)
F 1997, F 1999, F 2004, F 2005, F 2008, F 2009

CAS CH112 Intensive General and Quantitative Analytical Chemistry
Undergraduate Honors Course (2nd semester)
S1998, S 2000, S 2005, S 2006

CAS CH225 Mathematical Methods for Chemists
Undergraduate Course
F 2016

CAS CH351 Physical Chemistry I
Undergraduate Course
S 2001 (taught as CAS CH352 Physical Chemistry II)

CAS CH352 Physical Chemistry II
Undergraduate Course
S 2013, S 2015, S2016

CAS CH455 Advanced Computational Chemistry
Undergraduate Course
S 1997, S 2004 (cross-listed with GRS CH752 or GRS CH656)

Graduate Teaching in Theoretical and Computational Science

GRS CH655 Statistical Mechanics
Graduate Course (formerly GRS CH653)
F 1991, F 1992, F 1994, F 2000, F 2001, F2014

GRS CH656 Statistical Mechanics II
Graduate Course
S 2004

GRS CH658 Chemical Kinetics and Dynamics
Undergraduate/Graduate Course
S 2008, F 2012 (cross-listed with CAS CH458 in S 2008)

GRS CH752 Computational Chemistry and Biophysics
Graduate Course
S 1997

Elementary Science and Mathematics Education

This IS Rocket Science (8 week course)
Lincoln After School Program, William H. Lincoln Elementary School
F 2002, S 2003, S 2004, F 2004, S 2005

Magic: The After School Gathering (8 week course)
Lincoln After School Program, William H. Lincoln Elementary School
F 2002, S 2003, F 2003, S 2004, S 2005

Blast Off! (science camp)
Telluride Academy, Telluride, Colorado
U 2012, 2013, 2015, 2016

Graduate Education - Training Future Faculty and Research Scientists

GRS CH801 Graduate Research Methods and Scholarly Writing
F 2003

Sabbatical Leave

Bye Study Group on "Protein Biophysics"
Institute for Advanced Studies, Hebrew University, Jerusalem, Israel
F 1998

Bye Quantum Mechanics (CHEM557) and Special Topics in Biophysics (CHEM580)
Department of Chemistry and Biochemistry, Montana State University, Bozeman, Montana
F 2006, S 2007

Bye Teaching release for service as Chair
Department of Chemistry, Boston University, Boston, MA
F 2007, S2009, S2010, F2010, S2011, F2011, S2012

Invited Lectures (last 5 years)

29 June 2016 "Dynamics and thermodynamics in nanoconfined systems: Proteins and water," Workshop on Protein and Peptide Interactions in Cellular Environments, Telluride Science Research Center, Telluride, Colorado.

16 March 2016 "Complex role of solvation in micelle and reverse micelle environments," Symposium on Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events, American Chemical Society National Meeting, San Diego, California.

14 March 2016 "Probing the principles of amyloid protein aggregation," Symposium on Multiscales Chemistry, American Chemical Society National Meeting, San Diego, California.

11 January 2016 "Role of cholesterol in structure and function of lipid bilayers," Workshop on New Challenges for Theory in Chemical Dynamics, Telluride Science Research Center, Telluride, Colorado.

4 August 2015 "Toward a molecular theory of early and late events in monomer to amyloid fibril formation," Workshop on Protein Dynamics, Telluride Science Research Center, Telluride, Colorado.

21 July 2015 "Role of membrane in Amyloid Precursor Protein dimerization and cleavage," University of Tokyo (Hongo Campus), Tokyo, Japan.

10 July 2015 "Toward a molecular theory of early and late events in monomer to amyloid fibril formation," Symposium on Studying the Function of Soft Molecular Systems, Tokyo, Japan.

23 June 2015 "Dynamics and thermodynamics in nanoconfined systems: Proteins and water," Workshop on Dynamics in Complex Environments, Telluride Science Research Center, Telluride, Colorado.

19 May 2015 "Role of membrane in Amyloid Precursor Protein dimerization and cleavage," Boston University School of Medicine, Boston, Massachusetts.

11 May 2015 "Role of membrane in Amyloid Precursor Protein dimerization and cleavage," University of Texas, Austin, Texas.

26 March 2015 "Toward a molecular theory of early and late events in monomer to amyloid fibril formation," Symposium in Honor of Donald Truhlar, American Chemical Society National Meeting, Denver, Colorado.

8 December 2014 "Role of membrane in Amyloid Precursor Protein dimerization and cleavage," University of Kansas, Lawrence, Kansas.

1 December 2014 "Role of membrane in Amyloid Precursor Protein dimerization and cleavage," Brandeis University, Waltham, Massachusetts.

7 November 2014 "Role of sequence and membrane in Amyloid Precursor Protein structure and function," Academia Sinica, Taipei, Taiwan.

21 October 2014 "Probing the principles of protein aggregation," Department of Chemistry, Tufts University, Boston, Massachusetts.

16 October 2014 "Toward a molecular theory of early and late events in monomer to amyloid fibril formation," Department of Physics, Northeastern University, Boston, Massachusetts.

21 October 2014 "Structure and function of the transmembrane domain of Amyloid Precursor Protein and its role in the amyloid β protein aggregation pathway," International Conference on Computational Science and Engineering (ICCSE2014), Ho Chi Minh City, Vietnam.

5 June 2014 "Role of sequence and membrane in Amyloid Precursor Protein structure and function," Biopolymers Gordon Research Conference, Newport, Rhode Island.

1 April 2014 "Multiscale simulation of amyloid protein aggregation: Models and methods," Ontake Biophysics Symposium, Kiso-gun, Nagano, Japan.

14 March 2014 "The role of depletion forces in amyloid protein aggregation," Nagoya Symposium on Depletion Forces: 60th Anniversary of Asakura-Oosawa Theory, Nagoya University, Nagoya, Japan.

12 March 2014 "Multiscale modeling of amyloid protein aggregation," Science of Molecular Assembly and Biomolecular Systems Symposium, Nagoya University, Nagoya, Japan.

10 March 2014 "Probing the principles of amyloid formation," Workshop on Soft Molecular Systems, Kamisuwa, Nagano, Japan.

6 March 2014 "Multiscale simulation of transmembrane protein association," RIKEN, Wako, Japan.

6 February 2014 "Probing the principles of amyloid disease," a presentation to 40 high school students, Kozoji High School, Nagoya, Japan.

20-23 January 2014 "Structure, thermodynamics, and kinetics of amyloid formation," three lectures delivered to 34 graduate students and postdoctoral scientists, 13th KIAS Winter School on Protein Folding, High1 Resort, Kangwon Land, Korea.

16 December 2013 "A Lively Tour of the Periodic Table," a presentation to 250 middle school students as part of the Pinhead Scholars in the Schools program, Telluride Middle School, Telluride, Colorado.

16 December 2013 "A Lively Tour of the Periodic Table," a presentation to 120 middle school students as part of the Pinhead Scholars in the Schools program, Naturita Middle School, Naturita, Colorado.

21 November 2013 " Peptide homodimer structures in micelles and membranes," RIKEN Symposium on Biomolecular Simulation, RIKEN, Kobe, Japan.

19 November 2013 "Role of membrane in APP-C99 peptide dimerization and cleavage," International Conference on Molecular Simulation (ICMS2013): Large-Scale Molecular Simulations in Biology, Chemistry, and Physics, Kobe, Japan.

16 November 2013 "Probing the role of confinement and hydration in peptide folding and aggregation," Satellite Meeting of International Conference on Molecular Simulation (ICMS2013): Large-Scale Molecular Simulations in Biology, Chemistry, and Physics, Nagoya University, Nagoya, Japan.

25 October 2013 "Multiscale models for amyloid protein aggregation," Symposium Honoring Claudio Rebbi, Center for Computational Science, Boston University, Boston, MA.

3 October 2013 "When protein folding goes wrong: Probing the origins of amyloid disease," Department of Chemistry and Biochemistry, Providence College, Providence, RI.

4 June 2013 "Role of sequence and membrane in the transmembrane domain structure of Amyloid Precursor Protein," International Workshop on Computational and Theoretical Modeling of Biomolecular Interactions, Dubna, Russia.

9 May 2013 "Role of sequence and membrane in the transmembrane domain structure of Amyloid Precursor Protein," Department of Physics, Drexel University, Philadelphia, PA.

8 April 2013 "Role of sequence and membrane in the transmembrane domain structure of Amyloid Precursor Protein," Symposium on New Advances in Understanding Protein Folding, American Chemical Society National Meeting, New Orleans, Louisiana.

19 March 2013 "Role of sequence and membrane in the transmembrane domain structure of Amyloid Precursor Protein," Symposium on Protein Misfolding and Aggregation, American Physical Society National Meeting, Baltimore, Maryland.

8 March 2013 "Role of sequence and membrane in the transmembrane domain structure of Amyloid Precursor Protein," Department of Chemistry, University of Nevada, Reno, Nevada.

28 February 2013 "Role of sequence and membrane in the transmembrane domain structure of Amyloid Precursor Protein," Department of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia.

5 December 2012 "Role of sequence and membrane in the transmembrane domain structure of Amyloid Precursor Protein," Department of Biochemistry and Molecular Biology, University of Chicago, Chicago, Illinois.

27 July 2012 "The Soaring Science of Rip Roaring Rockets, by Projectile Professional – Dr. John Straub," Public outdoor science lecture that drew 50 children, ages 5 to 15, in Telluride, Colorado.

26 June 2012 "Role of sequence and membrane in the transmembrane domain structure of Amyloid Precursor Protein," Workshop on Protein Interactions in Cellular Environments, Telluride Science Research Center, Telluride, Colorado.

4 June 2012 "The role of hydration and confinement in protein folding and aggregation," Computational Biophysics to Systems Biology 2012 (CBSB12), University of Tennessee, Knoxville, Tennessee.

22 May 2012 "The role of hydration and confinement in protein folding and aggregation," CECAM Workshop on Anchoring Simulations to Experiments: Challenges for Understanding and Treating Alzheimer's Disease, Institute for Biological Physical Chemistry, Paris, France.

10 May 2012 "Dynamics of methionine ligand rebinding in cytochrome c," International Symposium on Multiscale Chemical Reacting Systems, Nagoya University, Nagoya, Japan.

3 April 2012 "When Protein Folding Goes Wrong: Probing the molecular origins of amyloid disease," Department of Chemistry (Phi Beta Kappa Lecturer), Denison University, Granville, Ohio.

17 February 2012 "A Lively Tour of the Periodic Table," Department of Chemistry (Phi Beta Kappa Lecturer), University of North Carolina, Greensboro, North Carolina.

10 February 2012 "When Protein Folding Goes Wrong: Probing the molecular origins of amyloid disease," Department of Chemistry (Phi Beta Kappa Lecturer), Gettysburg College, Gettysburg, Pennsylvania.

2 January 2012 "Dynamics of methionine ligand rebinding in cytochrome c," Workshop on New Challenges in Chemical Dynamics, Telluride Science Research Center, Telluride, Colorado.