
BIOGRAPHICAL SKETCH

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NAME Gerstman, Bernard Scott	POSITION TITLE Professor of Physics and Biophysics		
eRA COMMONS USER NAME GERSTMAN			
EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)</i>			
INSTITUTION AND LOCATION	DEGREE <i>(if applicable)</i>	YEAR(s)	FIELD OF STUDY
Stony Brook University	B.S.	1976	Physics
Princeton University	Ph.D.	1981	Physics/Protein Biophysics
University of Virginia	Post-Doc	1981-85	Physics/Biophysics

A. Personal Statement

My Ph.D. dissertation was on quantum tunneling in ligand binding to heme proteins. As a post-doctoral fellow, I worked on structure-function relationships in electron transfer proteins. My current research involves computational investigations of molecular species that are implicated in a variety of catastrophic neurological disorders such as Alzheimer's, cancer and Parkinson's. I am also using the techniques of non-linear dynamics to investigate the physics of protein folding.

B. Positions and Honors.

Positions and Employment

1981-1985 Post-Doctoral Research Associate, Department of Physics and Program in Biophysics, University of Virginia
1985-1991 Assistant Professor of Physics, Florida International University
1991-1998 Associate Professor of Physics, Florida International University
1998-present Professor of Physics and Biophysics, Florida International University

Other Experience and Professional Memberships

Summer, 1989 Visiting Scientist, ATT Bell Laboratories, Biophysics Division
Summer, 1991 Visiting Scientist, Princeton University

1978-present Member, American Physical Society
1998-2004 Chairman, Institutional Review Board, Florida International University
2004-present Program Review panel member for the American Institute of Biological Sciences

Honors

1976 Φβκ
1987 Young Investigator's Travel Award, American Physical Society
1991 President's Research Prize in the Natural Science and Mathematics, University of Virginia
1996 Excellence in Teaching Award, Florida International University
1999 Excellence in Research Award, Florida International University
2002 Excellence in Teaching Award, Florida International University
2006 Excellence in Research Award, Florida International University

C. Selected peer-reviewed publications (in chronological order).

1. P. P. Chapagain, J. L. Parra, B. S. Gerstman and Y. Liu, "Sampling of states for estimating the folding funnel entropy and energy landscape of a model alpha-helical hairpin peptide", *The Journal of Chemical Physics*, **127**, 075103, 1-7, 2007.
2. Y. Liu, P. P. Chapagain, J. L. Parra, and B. S. Gerstman, "Lattice model simulation of interchain protein interactions and the folding dynamics and dimerization of the GCN4 leucine zipper", *The Journal of Chemical Physics*, **128**, 045106, 1-10, 2008.
3. P. P. Chapagain, Y. Liu, and B. S. Gerstman, "The trigger sequence in the leucine zipper: α -helical propensity dependence of folding and dimerization", *The Journal of Chemical Physics*, **129**, 175103, 1-9, 2008.
4. B. S. Gerstman and P. P. Chapagain
Book Chapter: "Self-organizing Dynamics in Protein Folding", *Molecular Biology of Protein Folding, Part B*, Ed.: P. M. Conn, *Progress in Molecular Biology and Translational Science*, **84**, 1-37, 2008.
5. B. S. Gerstman and P. P. Chapagain
"Self-organizing Dynamics in Protein Folding"
Molecular Biology of Protein Folding, Part B, Ed.: P. M. Conn
Progress in Molecular Biology and Translational Science, **84**, 1-37, 2008.
6. Y. Liu, P. P. Chapagain, and B. S. Gerstman
"Stabilization of native and non-native structures by salt bridges in a lattice model of the GCN4 leucine dimer"
The Journal of Physical Chemistry B, Article ASAP
Publication Date (Web): December 28, 2009
The Journal of Physical Chemistry B, **114** (2), 796–803, 2010.
7. P. P. Chapagain, B. S. Gerstman, Y. Bhandari, and D. Rimal
"Free energy landscapes and thermodynamic parameters of complex molecules from non-equilibrium simulation trajectories"
Physical Review E, **83**(6), 061905, 2011.
8. T. Steckmann, Z. Awan, B. S. Gerstman, and P. P. Chapagain,
"Kinetics of Peptide Secondary Structure Conversion During Amyloid β -Protein Fibrillogenesis"
Journal of Theoretical Biology, **301**, 95–102, 2012.
9. R. H. Austin and B. S. Gerstman
"Physics of Cancer"
AIP Advances, **2**, 010901, 2012.
10. Y. R. Bhandari, P. P. Chapagain, and B. S. Gerstman
"Lattice model simulations of the effects of the position of a peptide trigger segment on helix folding and dimerization"
Journal of Chemical Physics, **137**, 105103, 2012.
11. I. E. Chemmama, A. C. Pelea, Y. R. Bhandari, P. P. Chapagain, and B. S. Gerstman,
"Structural propensities and entropy effects in peptide helix-coil transitions"
Physical Review E, **86**, 031915, 2012.

12. C. K. Regmi, Y. R. Bhandari, B. S. Gerstman, and P. P. Chapagain
“Exploring the diffusion of molecular oxygen in the red fluorescent protein mCherry using explicit oxygen molecular dynamics simulations”
The Journal of Physical Chemistry B, **117**(8), 2247-53, 2013.
13. Bernard S. Gerstman and Prem P. Chapagain
“Computational Investigations of Protein Folding to Engineer Amino Acids to Encourage Desired Supersecondary Structure Formation”
In: Protein Supersecondary Structures, 191-204, Ed. Alexander E. Kister,
Methods in Molecular Biology 932, ISBN 978-1-62703-064-9, ISSN 1064-3745,
Humana Press 2013, Springer New York.
14. P. Konold, C. K. Regmi, P. P. Chapagain, B. S. Gerstman, R. Jimenez
“Hydrogen Bond Flexibility Correlates with Stokes Shift in mPlum Variants”,
The Journal of Physical Chemistry B, **118**(11), 2940–2948, 2014.
15. J. B. GC, Y. R. Bhandari, B. S. Gerstman, and P. P. Chapagain
“Molecular Dynamics Investigations of the α -Helix to β -barrel Conformational Transformation in the RfaH Transcription Factor”
The Journal of Physical Chemistry B, **118**(19), 5101-8, 2014.

D. Research Support

Ongoing Research Support

2011-2015 Computational Investigations of Monomeric Variants of Red Fluorescent Proteins
NIH, PI: P. Chapagain, \$428,376.00

Completed Research Support (Last 10 Years)

2003-2007 “Laser Induced Shock Waves and Vaporization in Biological Systems and Material Science”
Air Force Office of Scientific Research, Sole PI: B. Gerstman, \$458,500.