
BIOGRAPHICAL SKETCH

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NAME Chapagain, Prem	POSITION TITLE Associate Professor		
eRA COMMONS USER NAME (credential, e.g., agency login) CHAPAGAIN			
EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable.)</i>			
INSTITUTION AND LOCATION	DEGREE <i>(if applicable)</i>	MM/YY	FIELD OF STUDY
Tribhuvan University, Kathmandu, Nepal	B. Sc.	06/96	Physics
Tribhuvan University, Kathmandu, Nepal	M.Sc.	12/98	Physics
Florida International University, Miami, FL	Ph.D.	08/05	Physics/Biophysics
Cornell University, Ithaca, NY	Postdoctoral	08/06	Dynamics of infectious diseases

A. Personal Statement

Over the last several years, my research has focused on protein dynamics and folding which involves applying computational and statistical mechanical techniques to understand how a protein folds to its biologically functional configuration. The ultimate goal of the research in this field is to understand and determine a set of rules that will guide the choice of amino acids necessary to create desired protein configurations. I have extensive research experience in computational investigations of protein dynamics, especially in applying Monte Carlo methods in reduced models and have recently been developing expertise in Molecular dynamics simulations. In the last few years, my research has expanded to include more biological aspects of protein dynamics such as protein-protein interactions, protein aggregation and fibril formation in neurodegenerative diseases. I have been focusing on the use computational investigations to design monomeric red fluorescent proteins (RFP) that have enhanced photostability and fluorescent properties. My research interests also include broadly related fields of biological physics such as mathematical modeling of the dynamics of infectious diseases, self-organization and complexity. The work proposed in this grant will allow us to further expand the research scope and make important contributions to the field. Several graduate and undergraduate students, including three minority female students, are currently carrying out research in biophysics under my supervision.

B. Positions and Honors

Positions and Employment

1998-2000 Assistant Lecturer, Tribhuvan University, Nepal
1999-2000 Medical Physicist, Bhaktapur Cancer Hospital, Nepal
2006-2012 Assistant Professor, Department of Physics, Florida International University, Miami, FL
2012- Associate Professor, Department of Physics, Florida International University, Miami, FL

Other Experience and Professional Memberships

1998- Life member, Nepal Physical Society
2003- Member, American Physical Society
2013- Member, Biophysical Society

Honors

1996 Shreepati Medal for Excellence in Education (Topped the list of BSc recipients, local), Nepal
1998 Distinction (Topped the list of MSc physics recipients from the entire country), Nepal

2004	Dissertation Year Fellowship, Florida International University, Miami, FL
2004	National Science Foundation (NSF) Travel Award (STATPHY22)
2008	Faculty Summer Research Award, Florida International University, Miami, FL
2010	Faculty Summer Research Award, Florida International University, Miami, FL
2012	American Physical Society International Travel award.

C. Selected Peer-reviewed Publications

1. GC JB, Bhandari YR, Gerstman BS, and **Chapagain PP** "Molecular Dynamics Investigations of the α -Helix to β -Barrel Conformational Transformation in the RfaH Transcription Factor" *Journal of Physical Chemistry B* 118, 5101-5108 (2014).
2. Regmi CK, Bhandari YR, Gerstman BS and **Chapagain PP** "Exploring the diffusion of molecular oxygen in the red fluorescent protein mCherry using explicit oxygen molecular dynamics simulations" *Journal of Physical Chemistry B* 117, 2247-2253 (2013).
3. Steckmann T, Awan Z, Gerstman BS, and **Chapagain PP**. "Kinetics of peptide secondary structure conversion during amyloid-beta protein fibrillogenesis" *Journal of Theoretical Biology* 301, 95-101 (2012).
4. Laurent AD, Mironov VA, **Chapagain PP**, Nemukhin AV and Krylov, AI "Exploring Structural and optical properties of fluorescent proteins by squeezing: Modeling high-pressure effects on the mStraberry and mCherry red fluorescent proteins" *Journal of Physical Chemistry B* 116, 12426-12440 (2012).
5. **Chapagain PP**, Regmi CK, Castillo W. "Fluorescent protein barrel fluctuations and oxygen diffusion pathways in mCherry", *Journal of Chemical Physics* 135, 235101 (2011).
6. **Chapagain PP**, Gerstman BS. Excluded volume entropic effects on protein unfolding times and intermediary stability. *Journal of chemical physics* 120, 2475-81 (2004).
7. **Chapagain PP**, Parra JL, Gerstman BS, Liu Y. Sampling of states for estimating the folding funnel entropy and energy landscape of a model alpha-helical hairpin peptide. *Journal of chemical physics* 127, 075103 (2007).
8. **Chapagain PP**, Liu Y, Gerstman BS. The trigger sequence in the GCN4 leucine zipper: alpha-helical propensity and multistate dynamics of folding and dimerization. *Journal of chemical physics*. 129,175103 (2008).
9. Liu Y, **Chapagain PP**, Gerstman BS. Stabilization of native and non-native structures by salt bridges in a lattice model of the GCN4 leucine dimer. *Journal of Physical Chemistry B* 114, 796-803 (2010).
10. **Chapagain PP**, Gerstman BS. Removal of kinetic traps and enhanced protein folding by strategic substitution of amino acids in a model alpha-helical hairpin peptide. *Biopolymers* 81, 167-78 (2006).

D. Research Support

Ongoing Research Support

1SC3GM096903 (PI: Chapagain) 7/1/2011 – 6/30/2015

NIH/NIGMS \$75,000 direct/year

Computational Investigations of Monomeric Variants of Red Fluorescent Proteins

The major goal of this research is to investigate protein barrel fluctuations and oxygen permeability in monomeric red fluorescent proteins using molecular dynamics simulations.

Completed Research Support

Faculty Summer Research Support, FIU

06/01/08-08/31/08

Effects of trigger sequence on folding and dimerization of GCN4 Leucine Zipper