

# Shachi S. Gosavi

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## EDUCATION

Ph.D., Chemical Physics. Aug, 2002  
California Institute of Technology, Pasadena.  
Thesis Title: Electron Transfer at Metal Surfaces  
Advisor: Professor Rudolf A. Marcus

M.Sc., Chemistry March, 1995  
Indian Institute of Technology, Bombay, India.

## CURRENT EMPLOYMENT AND RESEARCH

*Postdoctoral Researcher* May 2003 – present  
with Prof. J. N. Onuchic and Prof. P. A. Jennings  
Dept. of Physics, Univ. of California, San Diego  
Research on protein folding dynamics and the relation between folding and function in proteins. Focus on the  $\beta$ -trefoil proteins, in particular IL1 $\beta$ .

## SCIENTIFIC AND ACADEMIC EMPLOYMENT

*Research Assistant* Dec 1995 – Aug 2002.  
California Institute of Technology  
Study of various aspects of electron transfer at gold and platinum interfaces: dependence of rate constants on density of states in the metals, temperature dependence of rate constants, inverse photoemission at metal solution interfaces. We developed a method, which uses the Z-transform, to calculate the tight binding wavefunction of a metal with a surface.

*Research Assistant* June 1994 – Aug 1995  
with Dr. B. L. Tembe, IIT, Bombay.  
Ran molecular dynamics simulations for calculating the diffusion coefficients of super-ionic conductors. Debugging and addition to a MD program.

*Teaching Assistant*

Sept 1995 – June 2000.

California Institute of Technology

Introductory General Chemistry (Ch 1abc)

Equilibrium Statistical Mechanics (Ch 164)

Nonequilibrium Statistical Mechanics (Ch 165)

Introduction to Electron Transfer (Ch 221)

## TALKS AND POSTERS

*Informal Seminar on Mathematics and Biochemistry-Biophysics*

Dept. of Mathematics, Univ. of California San Diego, La Jolla, CA, May, 2008.

Presented a talk on “Protein Folding, Topological Frustration and Biological Function.”

*Department of Chemistry Seminar*

Indian Institute of Technology, Mumbai, India, Mar, 2008.

Presented a talk on “Function modulates the  $\beta$ -trefoil folding landscape.”

*Maria Goepfert Mayer Symposium, American Chemical Society*

San Diego, CA, Oct, 2007.

Presented a talk on “Functional regions complicate folding in simulations of interleukin-1 $\beta$ .”

*Center for Theoretical Biological Physics Workshop: Protein Dynamics: Going from In Vitro to In Silico*

CTBP, Univ. of California San Diego, La Jolla, CA, May 12th and 13th, 2007.

Presented the introductory session on “Introduction to simulation fundamentals and simplified models of proteins.”

*Center for Theoretical Biological Physics Seminar*

CTBP, Univ. of California San Diego, La Jolla, CA, January, 2007.

Presented a talk on “Slow Folding, Topological Frustration and Function: A case study of the  $\beta$ -trefoil family of proteins.”

*Biocomputation and Bioinformatics Constellation Seminar*

Rensselaer Polytechnic Institute, Troy, New York, August, 2006.

Presented a talk on “Folding, Topological Frustration and Function: A folding study of the  $\beta$ -trefoil family of proteins.”

*Protein Folding Dynamics*

Gordon Conference

Organised by Dr. Jane Clarke and Dr. Charles Brooks III, Ventura, California, Jan, 2006.

Presented a poster on “Folding, Topological Frustration and Function in IL1 $\beta$ .”

Awarded a best poster award.

*ONR Electrochemistry Section Review*

Annapolis, Maryland, March, 2004.

Presented a talk on “Inverse Photoemission at Metal Electrodes.”

PUBLICATIONS

P. C. Whitford, J. K. Noel, S. Gosavi, A. Schug, K. Y. Sanbonmatsu and J. N. Onuchic, “An All-atom Structure-Based Potential for Proteins: Bridging Minimal Models with All-atom Empirical Forcefields,” *PROTEINS: Struct. Funct. Bioinformatics*, doi:10.1002/prot.22253.

B. Andrews, S. Gosavi, J. M. Finke, J. N. Onuchic and P. A. Jennings, “The Multiple Basin Landscape in GFP Folding,” *Proc. Natl. Acad. Sci.*, 105, p. 12283, 2008.

S. Gosavi, P. C. Whitford, P. A. Jennings and J. N. Onuchic, “Extracting function from a  $\beta$ -trefoil folding motif,” *Proc. Natl. Acad. Sci.*, 105, p. 10384, 2008.

P. C. Whitford, S. Gosavi, and J. N. Onuchic, “Conformational transitions in adenylate kinase: Allosteric communication reduces misligation family,” *J. Biol. Chem.*, 283, p. 2042, 2008.

L. L. Chavez, S. Gosavi, P. A. Jennings and J. N. Onuchic, “Multiple routes lead to the native state in the energy landscape of the  $\beta$ -trefoil family,” *Proc. Natl. Acad. Sci.*, 103, p. 10254, 2006.

S. Gosavi, L. L. Chavez, P. A. Jennings and J. N. Onuchic, “Topological Frustration and the folding of Interleukin-1 $\beta$ ,” *J. Mol. Biol.*, 357, p. 986, 2006.

S. Gosavi and R. A. Marcus, “Inverse Photoemission at Metal Electrodes,” *Electrochim. Acta.*, 40, p. 3, 2003.

S. Gosavi, Y. Q. Gao, and R. A. Marcus, “Temperature Dependence of the Electronic Factor in the Nonadiabatic Electron Transfer at Metal and Semiconductor Electrodes,” *J. Electroanal. Chem.*, 500, p. 71, 2001.

S. Gosavi and R. A. Marcus, “Nonadiabatic Electron Transfer at Metal Surfaces,” *J. Phys. Chem. B*, 104, p. 2067, 2000.

*In preparation:*

S. Gosavi, K. Hailey, D. Capraro, S. Werner, L. L. Chavez, A. Hoffmann, P. A. Jennings and J. N. Onuchic, “Inferring function from protein structural differences,” in preparation.

D. Capraro, M. Roy, S. Gosavi, J. C. Covalt Jr., J. N. Onuchic and P. A. Jennings, “Modulating the Folding Routes of Interleukin-1 $\beta$  by Circular Permutation,” in preparation.

W. D. Anderson, S. Gosavi, M. Roy, G. Melancini, J. N. Onuchic and P. A. Jennings,  
“Surface Mutations Modulate Distal Effects in Interleukin-1 $\beta$ ,” in preparation.

#### AWARDS

Best poster award: Protein Folding Dynamics Gordon Conference, 2006.

Title: “Folding, Topological Frustration and Function in IL1 $\beta$ .”

La Jolla Interfaces in Science Fellowship, Burroughs Wellcome Fund: 2004 - Present.

National Talent Search Scholarship: 1988 - 1995.

Second in the M.Sc. graduating class of 1995, Indian Institute of Technology, Bombay.