

# Curriculum Vitae

## Hugh Nymeyer

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## Education:

- Ph.D. In physics from the University of California, San Diego, CA, 2001. Thesis entitled *Computational Studies of Protein Folding* under the supervision of Prof. José N. Onuchic.
- B.S. In physics & mathematics from Calvin College, Grand Rapids, MI, 1994.

## Employment/Professional Experience:

- 2001 – present Directors Funded Post-doctoral Fellow, Los Alamos National Laboratory.
- 1996 – 2001 Research Assistant at the University of California, San Diego.
- 1994 – 1996 Teaching Assistant at the University of California, San Diego.
- 1993 – 1994 Summer Research Assistant at Calvin College, Grand Rapids, MI.

## Current Interests:

I am currently interested in the development of enhanced sampling methods and their application to simulations of biological systems. Most enhanced sampling methods have been developed to circumvent the critical slowing down seen at discontinuous phase transitions or in glassy systems. Many biological systems exhibit both these features. For example, the globular proteins have cooperative folding/unfolding transitions as well as frustrated interactions and large enthalpic barriers, which produce a broad range of relaxation times. I am currently involved in using enhanced sampling methods to study the enthalpic and entropic forces guiding protein folding, the use of reduced coordinates to describe folding transitions, structural changes in lipid bilayers, and the interactions of peptides with lipid bilayers.

## Publications:

Hugh Nymeyer & Angel E. García, **Replica exchange calculations of the TRPcage protein in explicit solvent**, *In preparation*.

Hugh Nymeyer, Thomas B. Woolf & Angel E. García, **Folding is not required for insertion: Replica exchange calculations for an alpha-helical peptide in an explicit lipid bilayer**, *J. Mol. Biol.*, *submitted* (2003).

Hugh Nymeyer & Angel E. García, **How well does the GB/SA approximation describe the folding equilibrium of alpha helical peptides? -- A side by side comparison with explicit solvent simulations**, *Proc. Nat'l Acad. Sci. USA*, *accepted for publication* (2003).

Hugh Nymeyer, S. Gnanakaran, & Angel E. García, **Atomic simulations of peptide and protein folding equilibrium using the replica exchange algorithm**, *Methods in Enzymology*, accepted for publication (2003).

S. Gnanakaran, H. Nymeyer, J. Portman, K. Y. Sanbonmatsu & A. E. García, **Peptide folding simulations**, *Curr. Opin. Struct. Biol.*, **13**(2), 168-74 (2003).

J. Chahine, H. Nymeyer, V. B. P. Leite, N. D. Socci & J. N. Onuchic, **Specific and non-specific collapse in protein folding funnels**, *Phys. Rev. Lett.*, **88**(16), 168101-8101 (2002).

Cecilia Clementi, H. Nymeyer & J. N. Onuchic, **Topological and energetic factors: What determines the structural details of the transition state ensemble and "en-route" intermediates for protein folding? An investigation for small globular proteins**, *J. Mol. Biol.*, **298**(5), 937-953 (2000).

Hugh Nymeyer, N. D. Socci & J. N. Onuchic, **Landscape approaches for determining the ensemble of folding transition states: Success and failure hinge on the degree of frustration**, *Proc. Nat'l Acad. Sci. USA*, **97**(2), 634-9 (2000).

J. N. Onuchic, H. Nymeyer, A. E. García, J. Chahine & N. D. Socci, **The energy landscape theory of protein folding: Insights into folding mechanisms and scenarios**, *Adv. Prot. Chem.*, **53**, 87-152 (2000).

H. Nymeyer, A. E. García & J. N. Onuchic, **Energy vs. native fold: Determinants of the folding transition state structure**, *Proc. Nat'l Acad. Sci. USA*, **95**(11), 5921-8 (1998).

N. D. Socci, H. Nymeyer & J. N. Onuchic, **Exploring the protein folding funnel landscape**, *Physica D*, **107**, 366-382 (1997).

S. L. Haan, B. Langdon, D. Streutker & H. Nymeyer, **Formation and collapse of a bound dressed state in strong-field, near-threshold photodetachment**, *Laser Phys.*, **7**(1), 115-8 (1997).

D. Zuo, T. Vos, H. Nymeyer, L. Reynolds, H. S. Schnyders, & J. B. Van Zytveld, **Electronic properties of the liquid alloys AlCa and AlBa**, *J. Non-Crystal. Sol.*, **207**(1), 328-31 (1995).

S. L. Haan, M. Bolt, H. Nymeyer & R. Grobe, **Effects of positive-ion resonances in photoionization of neutral atoms**, *Phys. Rev. A*, **51**(6), 4640-51 (1995).

## REFERENCES for Hugh Nymeyer

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