

**Stony Brook University
The Graduate School**

Doctoral Defense Announcement

Abstract

Study of Biologically Relevant Phenomena Using Small Peptide Models

By

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Understanding protein structure and dynamics is a central and important problem in structural biology. Small model peptides are useful for studying this problem as they reduce the complexity involved in studying the folding of larger proteins while providing important insights into the formation of protein secondary structure. The small size of model peptides makes them particularly amenable to study by molecular dynamics (MD) simulations, which can provide atomic-level detail of peptide dynamics. When this data is used in conjunction with that from experiment it can be used to explain certain experimental results, or make predictions that can then be tested by experiment. Agreement with experimental results is an important benchmark for the validation of simulation results.

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Time: 3:00 PM

Place: Chemistry Building, Room 412

Program: Chemistry

Dissertation Advisor: Carlos Simmerling