Available Theoretical/Computational Research Projects

Isaac C. Sanchez

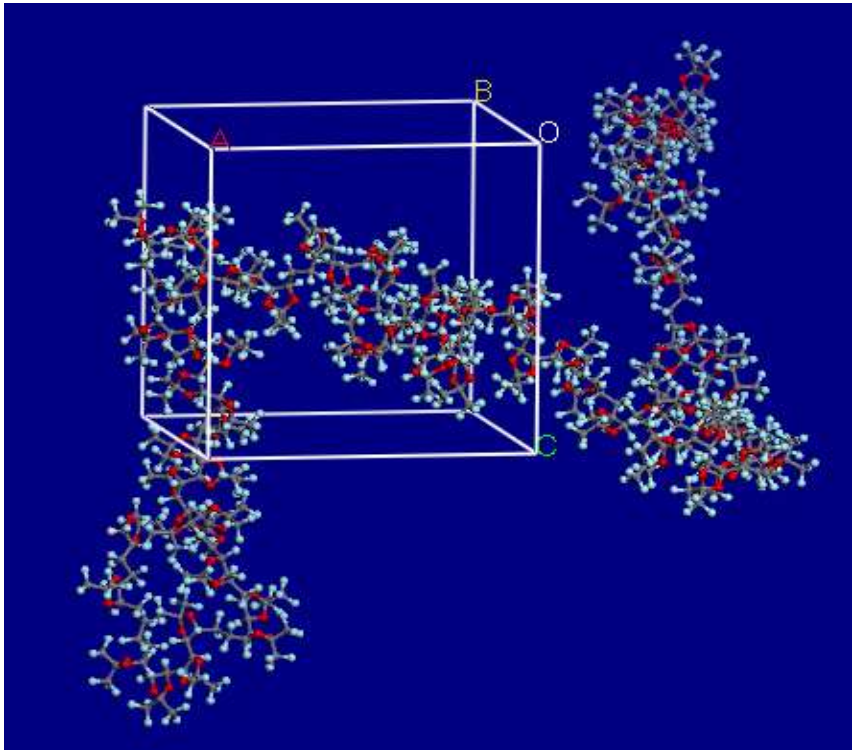
Statistical Thermodynamics of Polymers with a Biophysics Emphasis

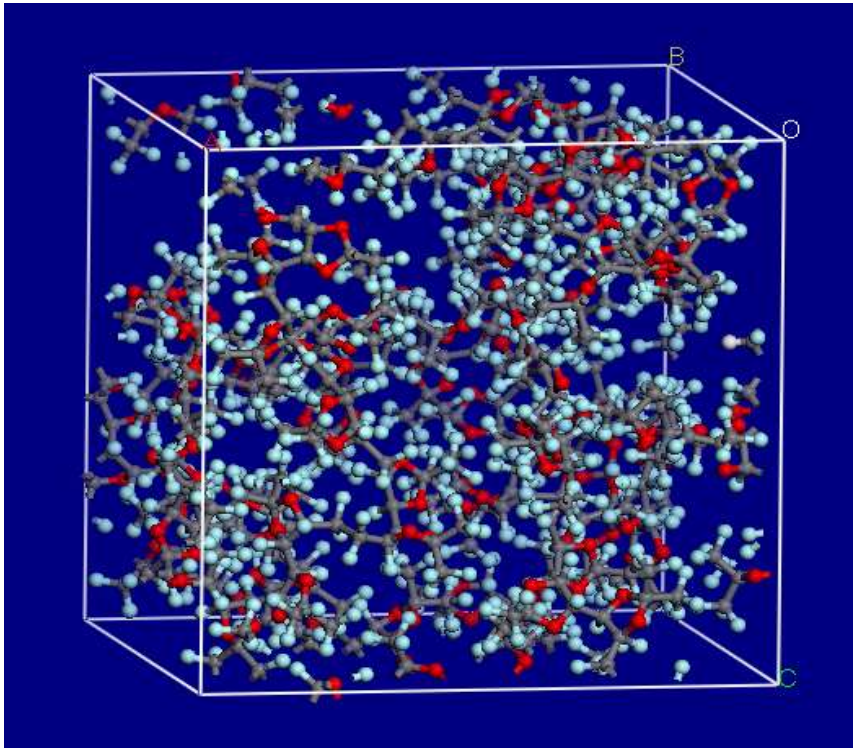
Continued development of Probabilistic Molecular Dynamics

Computer/Analytical models for the Cold Denaturation of Proteins

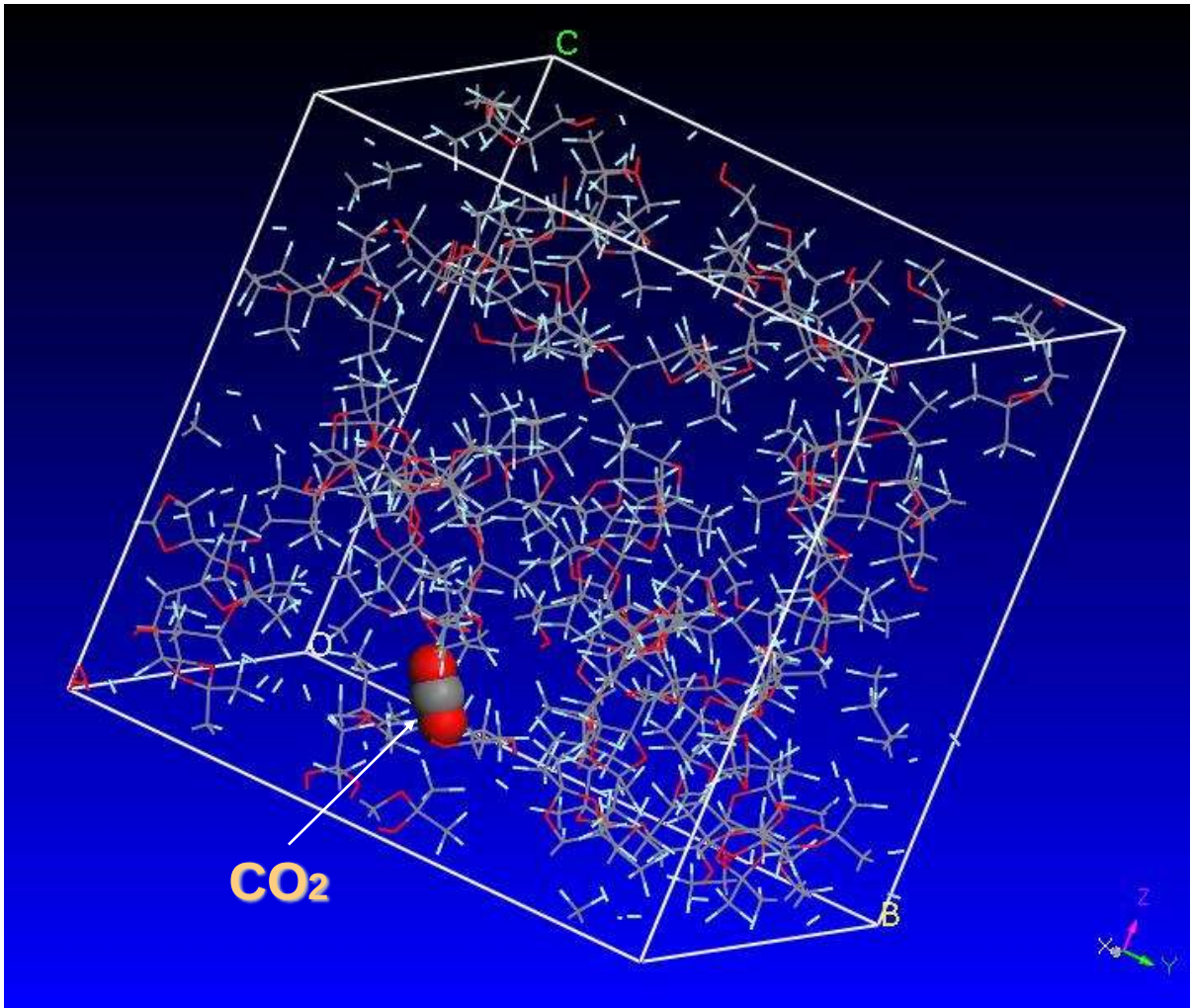
Computer simulation of cell aggregation & growth onto a tissue scaffold

Folding a Polymer Chain into a Simulation Box

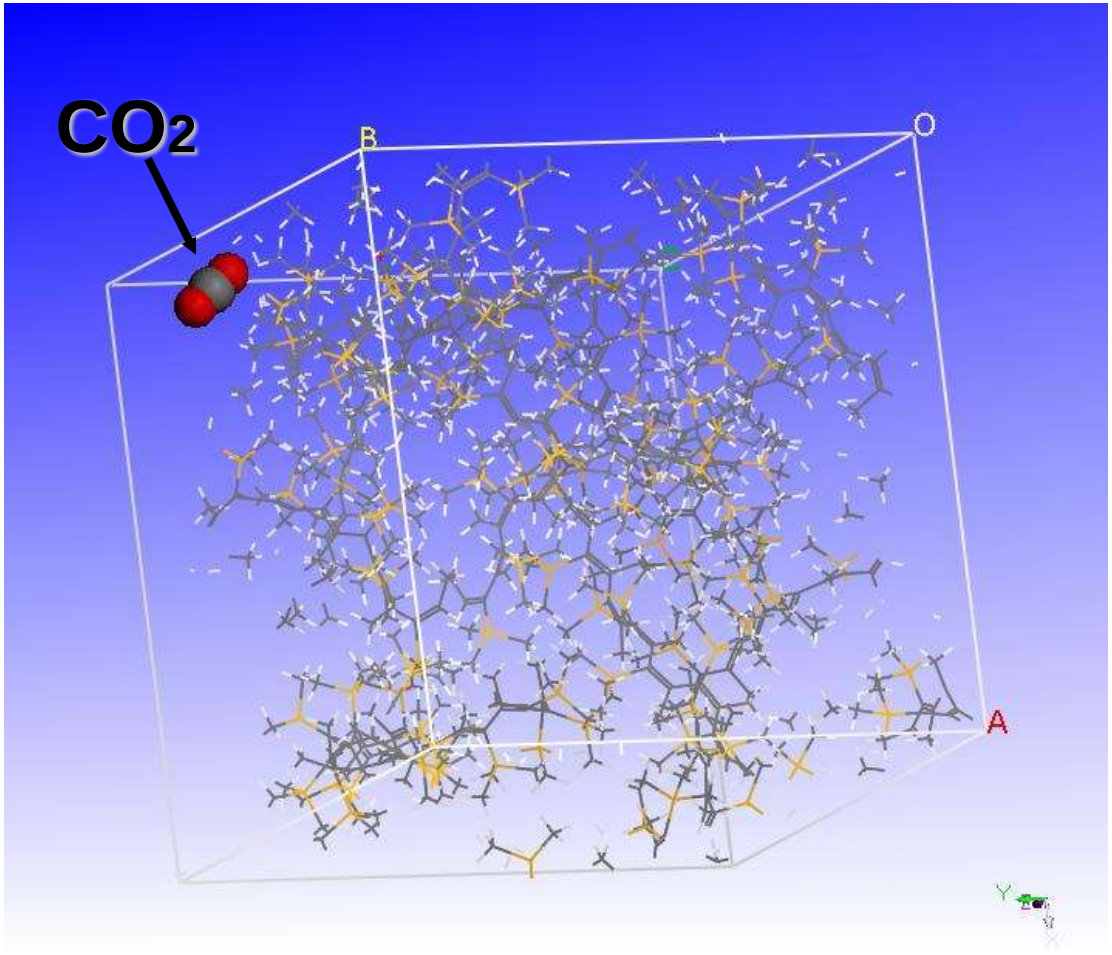




Diffusion by Probabilistic Molecular Dynamics



Solubility by Monte Carlo Simulation



Available Theoretical/Computational Research Projects

Isaac C. Sanchez

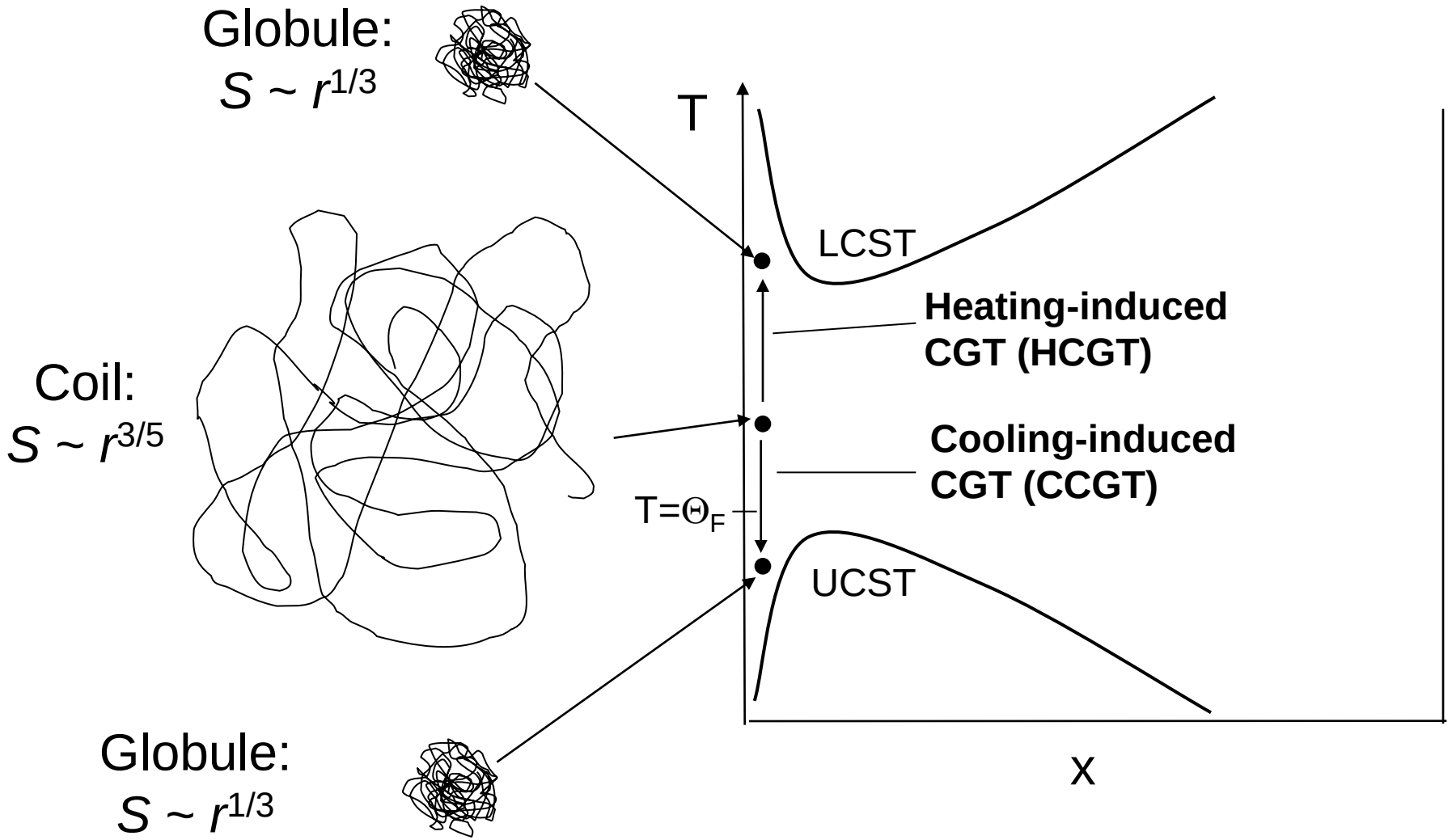
Statistical Thermodynamics of Polymers with a Biophysics Emphasis

Computer/Analytical models for the Cold Denaturation of Proteins

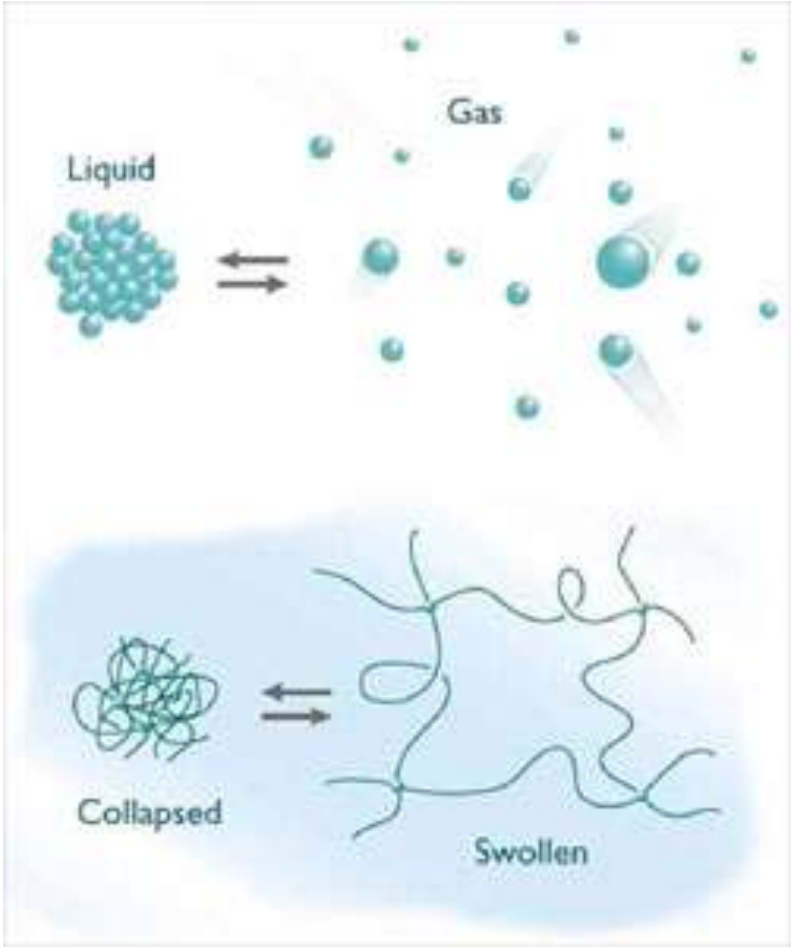
Computer simulation of cell aggregation & growth onto a tissue scaffold

Continued development of Probabilistic Molecular Dynamics

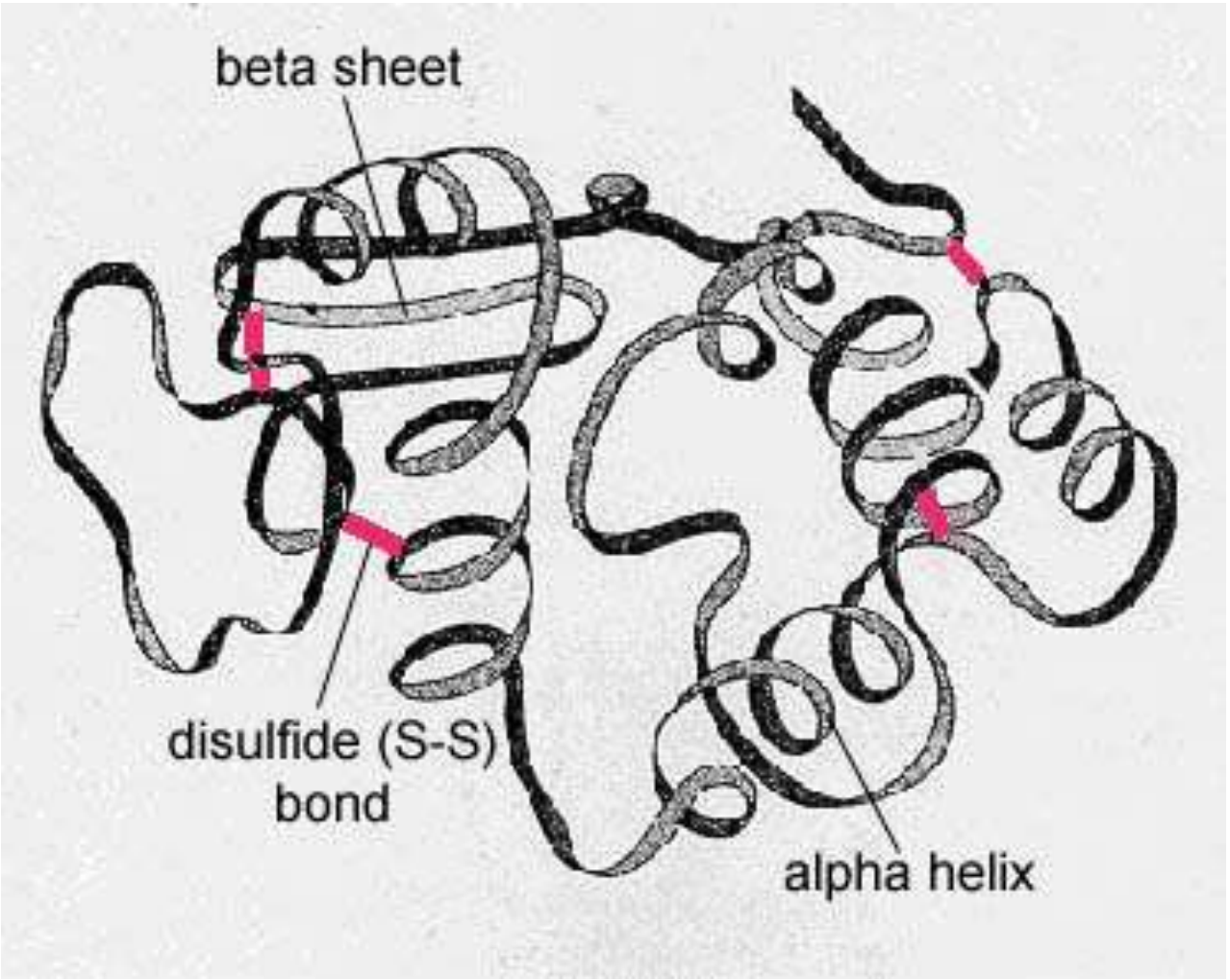
Coil-Globule Transitions



Similarity to Gas-Liquid Transition



Globular Protein Structure



Motivations

- Cold–denaturation of proteins
- Drug delivery applications

Smart Hydrogels

- Hydrogels are made by cross-linking a water soluble polymer.
- Expansion-contraction transition temperature is the approximately the same as the transition temperature of the uncross-linked polymer.
- Hydrogels can be made to be target specific.

The Dream

Imagine delivering a drug imbibed in a gel via the blood stream to a diseased body part or organ. On arrival the gel interacts with the diseased cells releasing the drug with the gel safely dissolving.

Recent PhD Titles

- Phase and Conformational Behavior of LCST-driven Stimuli Responsive Polymers
- Effects of Supercritical Fluids on Thin Polymer Films
- Empty Space and How Things Move Around in It
- Monte Carlo Studies of Polymer Chain Solubility in Water
- Exploring Solvent Properties of High Pressure CO2 via Computer Simulation
- Monte Carlo Approaches to the Protein Folding Problem

Selected Recent Publications

- "*Gas Diffusion in Glasses via a Probabilistic Molecular Dynamics"*
  Frank T. Wilmore and Isaac C. Sanchez, *J. Chem. Phys*. **126**, 234502, (2007) .

- "*Welding Immiscible Polymers with a Supercritical Fluid*,"
  Xiaochu Wang and Isaac C. Sanchez, *Langmuir* 23, 12192, 2007

- "*Structural, Sorption and Transport Characteristics of an Ultrapermeable Polymer*," Xiao-Yan Wang, Anita Hill, Benny D. Freeman, & Isaac C. Sanchez, *J. Membrane Sci.,* **314,** 15, (2008).

- *"A Model for a Thermally Induced Polymer Coil-to-Globule Transition,"*
  David S. Simmons and Isaac C. Sanchez, *Macromolecules,* **41,** 5885 (2008).

- *"On the Asymptotic Properties of a Hard Sphere Fluid,"*
  Isaac C. Sanchez and Jang S. Lee, , *J. Phys. Chem. B*, **113**, 15572-15580, (2009).

- "*Pressure Effects on Polymer Coil-Globule Transitions near an LCST"*
  David S. Simmons and Isaac C. Sanchez, *Macromolecules* **43**, 1571–1574 (2010).