Available Theoretical/Computational Research Projects

Isaac C. Sanchez

Statistical Thermodynamics of Polymers with a Biophysics Emphasis

- Continued development of "Computational Structural Spectroscopy" of Proteins and RNA (with Lydia Contreras-Martin)
- Computer/Analytical models of Stimuli Responsive Hydrogels
- Computer simulation of cell aggregation & growth onto a tissue scaffold (with Christine Schmidt)

Computational Structural Spectroscopy (CSS)

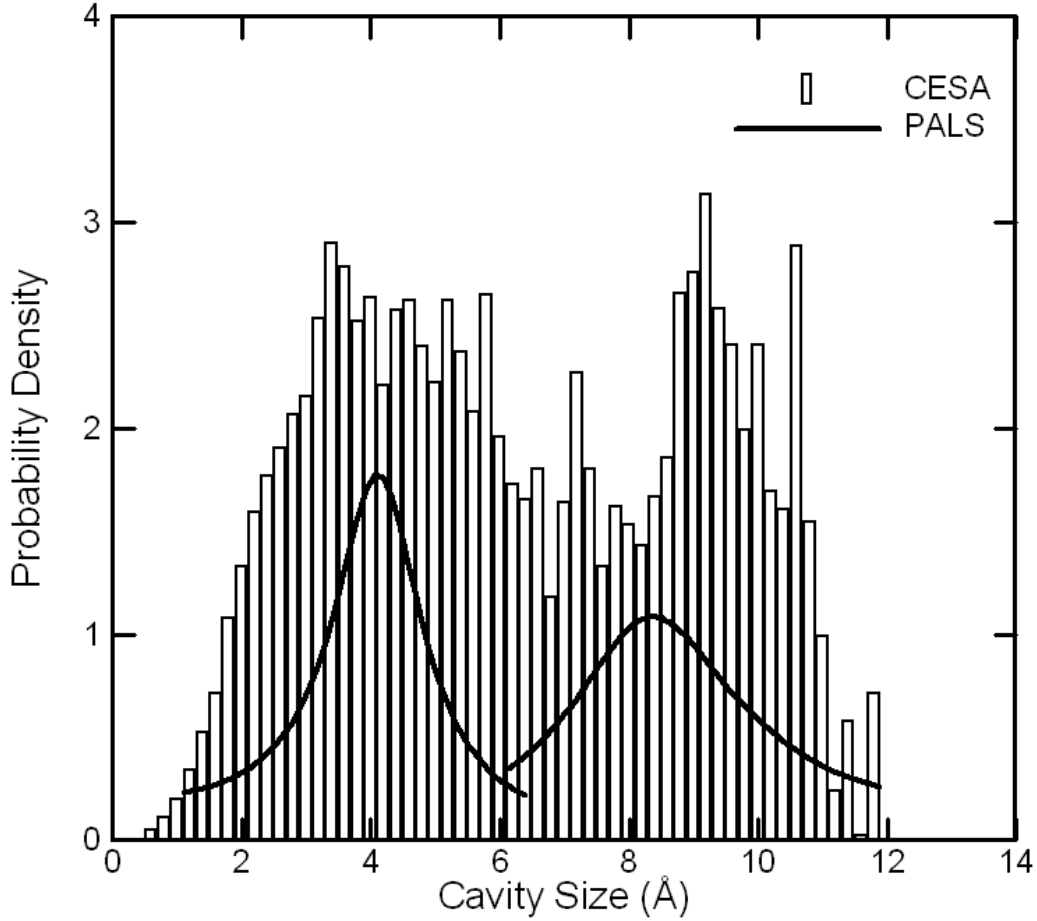
A new Monte Carlo method, based on the potential energy landscape of a globular protein, can characterize the void structure within a protein. This algorithm produces a characteristic "spectrum" for the cavity size distribution as well as a size spectrum of percolating and non-percolating paths through a protein.

For many proteins, it is widely believed that void structure plays an important role in function.

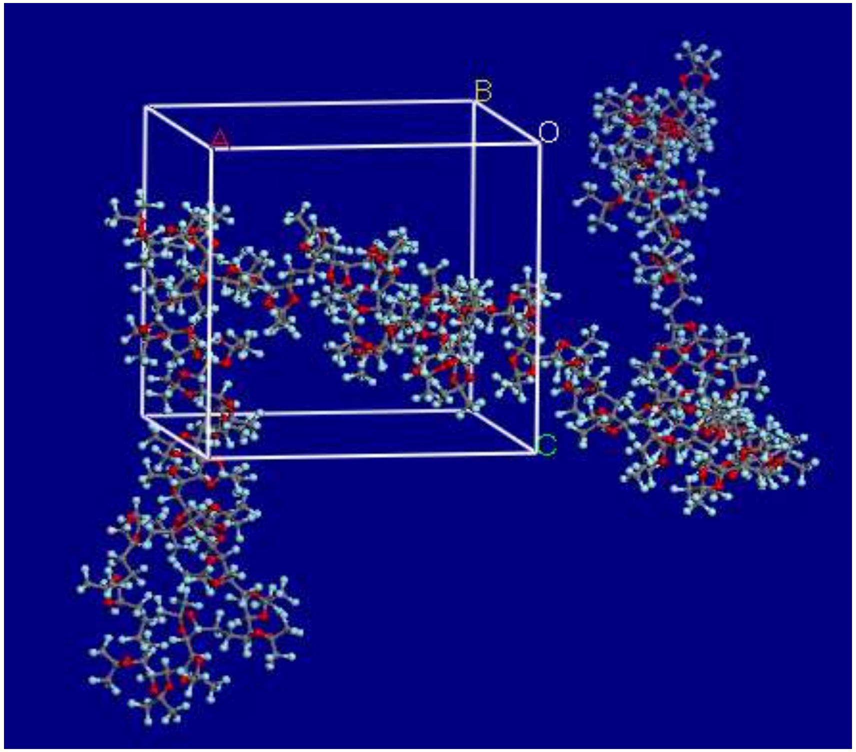
Future objectives: Map out optimal diffusion pathways for ions (e.g., Ca^{++}) and gas molecules such as O_2 and CO_2 within the void structure of a globular protein. Provide computer visualizations of protein void structure.

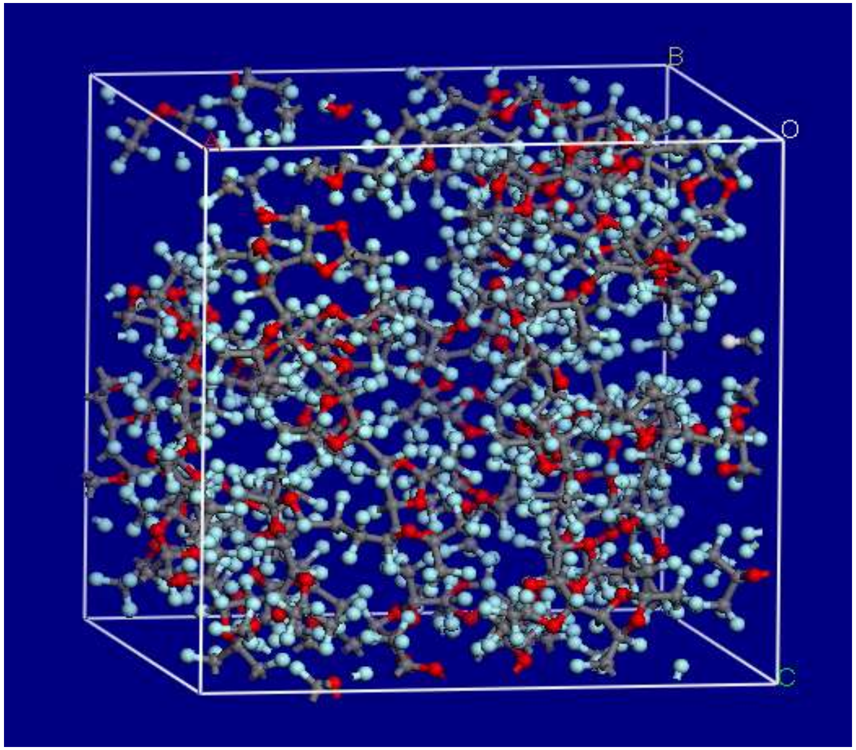
CSS of an amorphous polymer

[*Polymer*, **52**, 2244-2254, 2011]



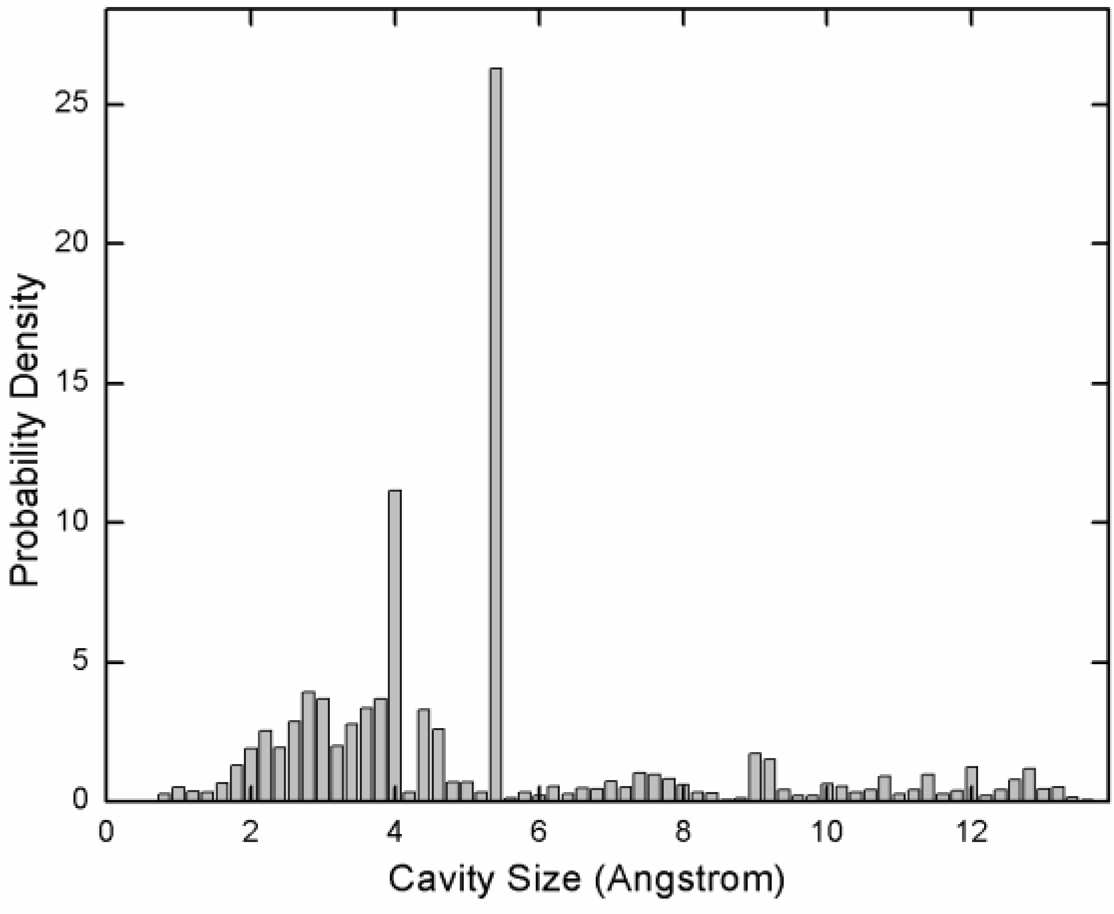
Folding a Polymer Chain into a Simulation Box



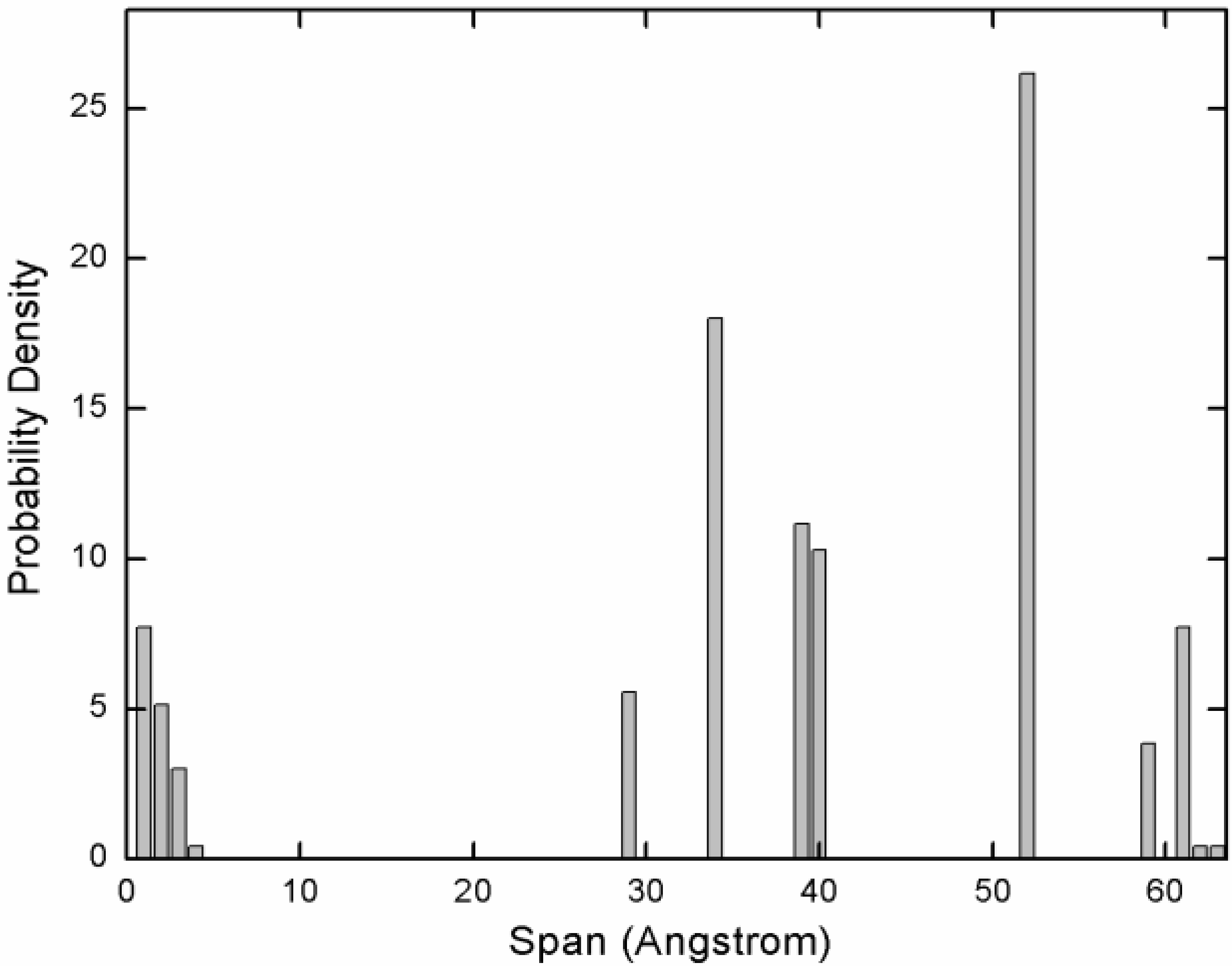


Structure of Aquaporin 2C32

Cavity Size Distribution in Aquaporin



Percolation Path (Span) Spectrum for Aquaporin



Available Theoretical/Computational Research Projects

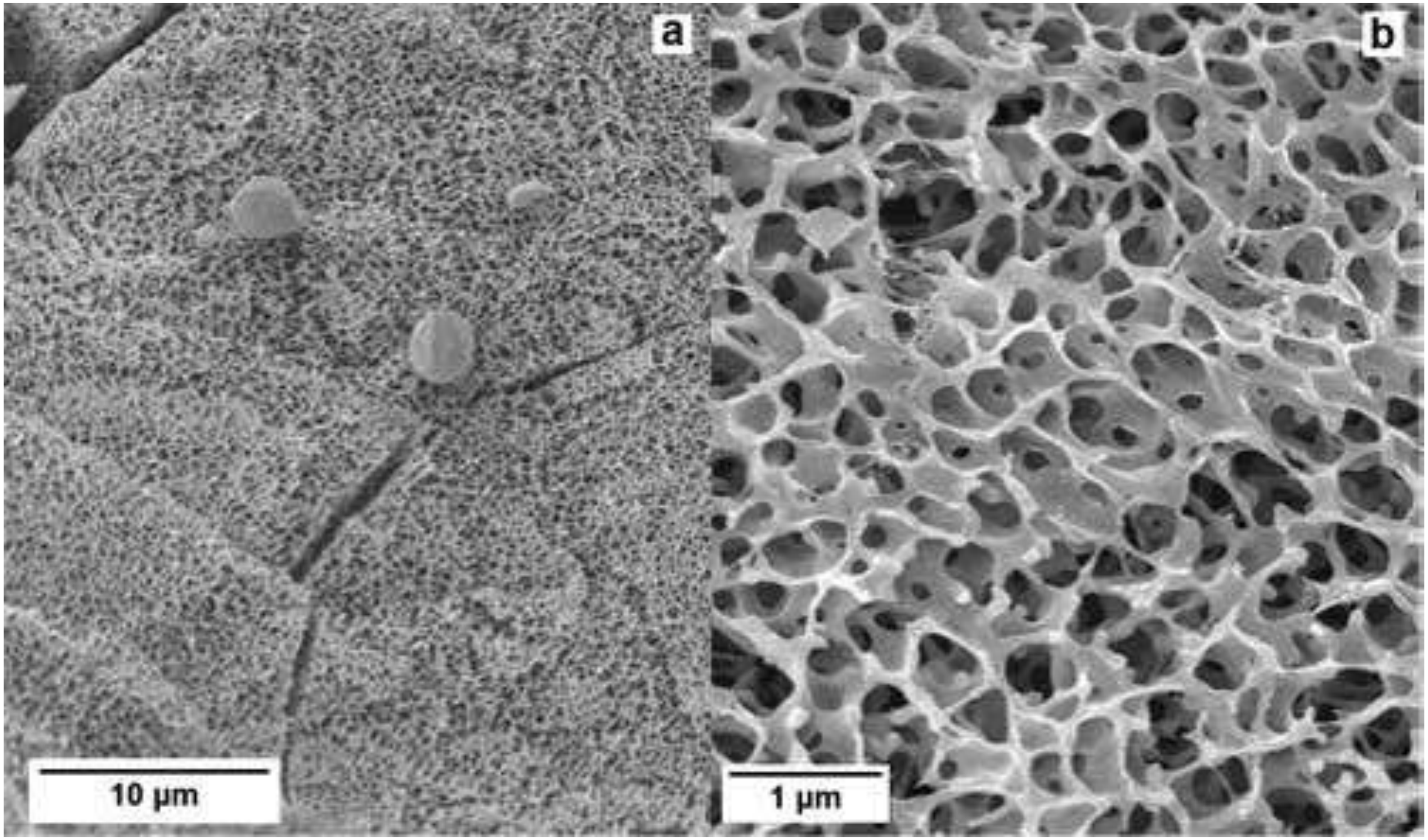
Isaac C. Sanchez

Statistical Thermodynamics of Polymers with a Biophysics Emphasis

- Continued development of "Computational Structural Spectroscopy" of Proteins and RNA (with Lydia Contreras-Martin)
- Computer/Analytical models of Stimuli Responsive Hydrogels
- Computer simulation of cell aggregation & growth onto a tissue scaffold (with Christine Schmidt)

Micrograph of a hydrogel

Micro-pores can open and close with changes in pH, salinity, specific ions, pressure, temperature, etc.



Motivation

Analytical/computer modeling the contraction-expansion mechanism of hydrogels

for drug delivery applications

The Dream

Stimuli responsive hydrogels can be made to be target specific.

Imagine delivering a drug imbibed in a micro-gel particle *via* the blood stream to a diseased body part or organ. On arrival the gel interacts with the diseased cells releasing the drug while the gel safely dissolves.

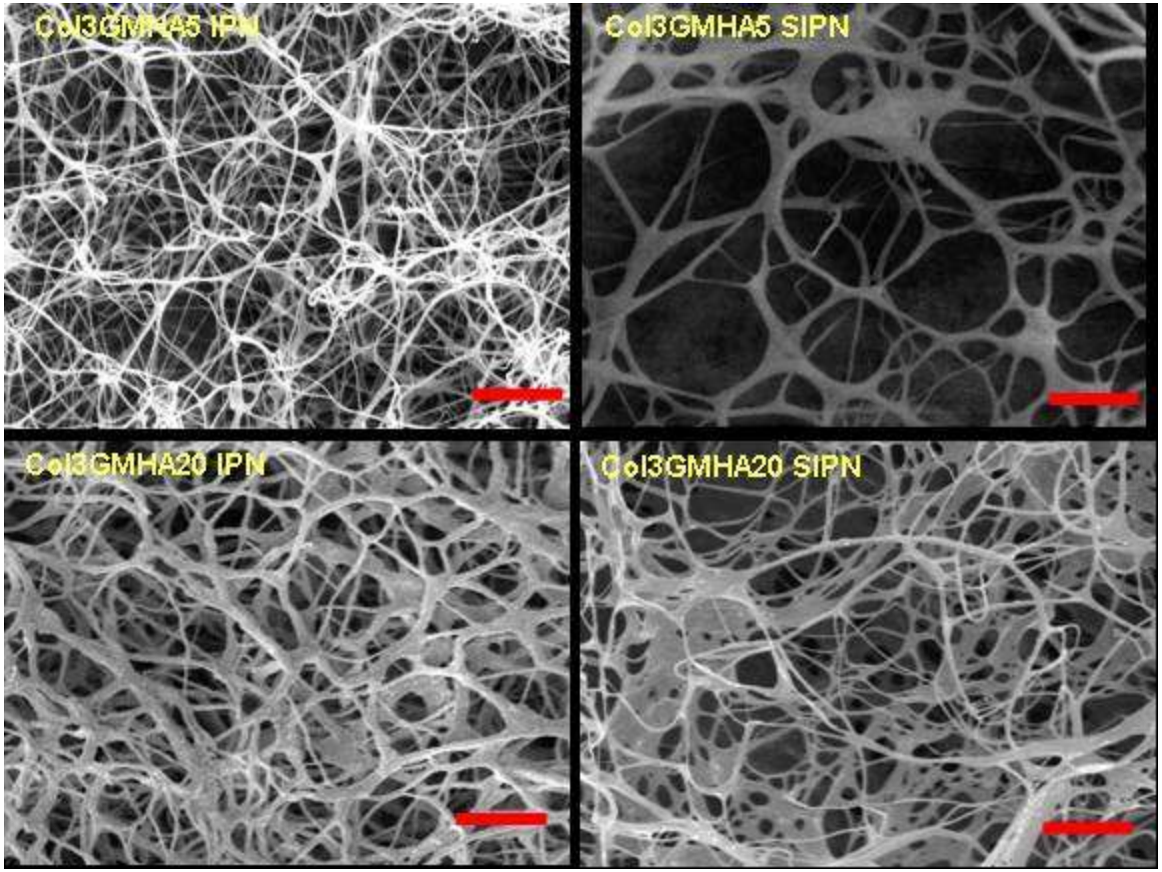
Available Theoretical/Computational Research Projects

Isaac C. Sanchez

Statistical Thermodynamics of Polymers with a Biophysics Emphasis

- Continued development of "Computational Structural Spectroscopy" of Proteins and RNA (with Lydia Contreras-Martin)
- Computer/Analytical models of Stimuli Responsive Hydrogels
- Computer simulation of cell aggregation & growth onto a tissue scaffold (with Christine Schmidt)

Hydrogels from the Schmidt lab as potential tissue scaffolds



Computer model for cell development in tissue scaffold

Determine the conditions that promote cell adhesion to the tissue scaffold.

A minimalist model is characterized by only 4 parameters: a cell size parameter, 2 parameters that measure the strength of cell-cell and cell-wall interactions, and a viscous drag parameter that determines the work energy required to move a cell through a viscous medium. Some variables that can be externally controlled are the surface-to-volume ratio of the porous scaffold, cell number density, and cell medium viscosity.

Selected Recent Publications

- "*Gas Diffusion in Glasses via a Probabilistic Molecular Dynamics"* F. T. Wilmore and I. C. Sanchez, J. *Chem. Phys*. **126**, 234502 (2007)
- *"On the Asymptotic Properties of a Hard Sphere Fluid,"* I. C. Sanchez and J. S. Lee, *J. Phys. Chem. B*, **113**, 15572-15580, (2009)
- *"Pressure Effects on Polymer Coil-Globule Transitions near an LCST"* D. S. Simmons and I. C. Sanchez, *Macromolecules* **43**, 1571–1574 (2010).
- *"Conductivity Mechanisms in a Composite of Chitosan-Silver Nanoparticles*," E. Prokhorov, *et. al*., *Mol. and Liq. Crystals*, **536,** 24-32, (2011).
- "*Cavity Size, Sorption, and Transport Characteristics of Thermally Rearranged Polymers*, Y. Jiang, *et. al*., *Polymer*, **52**, 2244-2254 (2011)
- *"Entropy of Living versus Non-living Systems,"* I. C. Sanchez, *J. Mol. Phys*., **2**, 654-57 (2011).