November 19, 2012
3:00 PM Livermore Center 101

Abstract

"Computational Modeling of the Void Structure in Polymeric Glasses and Globular Proteins"

Isaac C. Sanchez
Chemical Engineering Dept.
University of Texas
Austin, Texas

Within a polymer thin film, free-volume elements have a wide range of size and topology. This broad range of free-volume element sizes determines the ability for a polymer to perform molecular separations. Using atomistic models, cavity size (free volume) distributions were determined by a combination of molecular dynamics (MD) and Monte Carlo methods for 6 thermally rearranged (TR) polyimides and their precursors. Diffusion, solubility, and permeation of gases in TR polymers and their precursors were simulated at 308 K, with results that agree with experimental data. A similar methodology has been used to characterize the void structure within globular proteins. The method produces a spectrum of the empty cavities and channels within a protein and has been labeled ?computational spectroscopy.? Molecular dynamics provides a picture of structural changes with time. Since water molecules can occupy the void spaces, the MD simulation also reveals how water can move in out of a protein. Water channels also provide pathways for the migration of small molecules such as oxygen to the active site within the protein. Application to myoglobin and some of its mutants will be used to illustrate the methodology and its potential for drug design.