420 - Oxygen diffusion in water, alkanes, and lipid bilayers

An Ghysels[1], *an.ghysels@ugent.be, Richard M Venable*[2], *Richard W Pastor*[2], *Gerhard Hummer*[3]. *(1) Center for Molecular Modeling, Ghent University, Ghent, Belgium, (2) National Heart Lung and Blood Institute, National Institutes of Health, Bethesda, Maryland 20824, United States, (3) National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, Maryland 20824, United States*

Oxygen diffusion in the cellular medium and in lipid membranes is essential for aerobic life. We used molecular dynamics simulations to study the energetics and dynamics of the diffusive O2 transport in water, alkanes and lipid bilayers of different composition. From our simulations the underlying free energy surfaces and diffusion coefficients are determined both in homogeneous and isotropic neat water and alkane phases, and across inhomogeneous and anisotropic water-alkane interfaces and lipid membranes. Free energy surfaces and position-dependent diffusion tensors describing the oxygen transport within and across membranes of different lipid compositions are derived from intermediate time propagators analyzed with Bayesian inference. To enter into a lipid bilayer, oxygen needs to overcome a free energy barrier as it passes the head group region. Once inside the membrane, oxygen concentrates at the center, between the two leaflets, where also the local diffusivity is enhanced. Differences in the energetics and diffusivities between the various systems studied point to the underlying molecular mechanisms. The oxygen affinities and in-plane diffusivities are compared for a membrane with a lipid composition mimicking the inner mitochondrial membrane and for a POPC model membrane. This comparison sheds light on how aerobic life achieves an efficient oxygen delivery to cytochrome c oxidase, the terminal oxidase in mitochondria that drives cellular respiration.

Wednesday, April 10, 2013 02:30 PM
Membranes (01:30 PM - 04:45 PM)
Location: Morial Convention Center
Room: 356