Yale Institute for Nanoscience and Quantum Engineering

Friday- April 8, 2016

12:00 to 1:00 p.m.

BECTON SEMINAR ROOM

Light lunch will be served at 11:45 a.m.

Abbas Firoozabadi

Director, Reservoir Engineering Research Institute (RERI) in Palo Alto, California

"Molecular Structure of Petroleum Interfaces in Relation to Environmental Stewardship and Efficient Production"

Nanoscale, microscale, and ionic aggregation both in the bulk and interfaces are becoming increasingly viable in relation to efficient production of hydrocarbon resources as well the environmental stewardship. Use of small quantities of functional molecules has the potential to improve both efficiency and reduce environmental impact in hydrocarbon production. Salt concentration in the injected water may have a profound effect on improved oil recovery. The functional molecules in small quantities can reduce the need for harmful chemicals in flow assurance and safe production of natural gas considered by many as the transformational fuel. In relation to the effect of salt concentration, the understanding of the mechanisms despite some 500 papers on the subject is limited. Molecular structure at the fluid-fluid and fluid-solid interfaces would provide insight.

This presentation will cover a combination of MD simulations and basic concepts to compute aggregation of molecules and molecular structures. The structure of methane and propane hydrates are computed first; some 50 and 150 molecules are assembled to form the unit cells of methane and propane hydrates, respectively. In a more detailed demonstration, the contact angle in two petroleum fluid systems will be predicted as a function of NaCl concentration. Mica is the substrate. For the first time we demonstrate agreement from atomistic MD simulations of contact angle and lab measurements. We also show that the oil composition can result in non-monotonicity of contact angle with salt concentration in line with our recent measurements.

Fred Sigworth

Departments of Physiology and Biomedical Engineering, Yale University

"Atomic Structures of Biological Macromolecules from Electron Cryo-Microscopy"

Electron microscopy of proteins, DNA and other macromolecules has recently advanced to the point where near-atomic-resolution structures can be obtained without the requirement of crystallization or labeling of the specimen. Instead, individual copies of the macromolecule of interest are imaged in a layer of vitreous ice, and the resulting "single particle" images are analyzed to determine the orientation of each particle. Combining information from a set of 10^4 to 10^5 particle images, one can now obtain a 3D density map in which details at 3 Å or smaller scales can be resolved. I will describe the technical developments that have made possible this advance in resolution, and will discuss work in my laboratory on structures of membrane proteins using this technique.

Host: Professor Eric Altman