University of Minnesota
Driven to Discover℠

Department of Chemistry

Special Seminar

4:30 p.m. Monday, November 29 • 331 Smith Hall

Professor

Berend Smit

Department of Chemical and Biomolecular Engineering
University of California, Berkeley

Mesoscopic Simulations of Membranes: What is Special About Cholesterol?

Research interests:
The development and application of molecular simulation techniques that enable us to explore exciting and novel molecular solutions to problems in chemical engineering and physical chemistry that are inaccessible experimentally.

Website: http://cheme.berkeley.edu/faculty/smit/

Abstract

To gain insight into the lipid-mediated interactions between (trans)membrane proteins, we developed a mesoscopic model of a lipid bilayer with embedded proteins. This model is simulated using dissipative particle dynamics. Our calculations of the potential of mean force between these transmembrane proteins show that hydrophobic forces drive long-range protein-protein interactions and that the nature of these interactions depends on the length of the protein hydrophobic segment, on the three- dimensional structure of the protein, and on the properties of the lipid bilayer.

We also discuss the effect of cholesterol on these lipid-mediated protein-protein interactions. We propose a mechanism by which cholesterol affects protein interactions: protein-induced, cholesterol-enriched, or cholesterol-depleted lipid shells surrounding the proteins affect the lipid-mediated protein-protein interactions. Our calculations of the potential of mean force between proteins and protein clusters show that the addition of cholesterol dramatically reduces repulsive lipid-mediated interactions between proteins (protein clusters) with positive mismatch, but does not affect attractive interactions between proteins with negative mismatch.

Host: Professor Laura Gagliardi
Refreshments will be served prior to the seminar.