

Biological Membranes and Membrane Proteins Schedule (2019)

(The Santa Fe Conference, June 10th – June 13th, 2019)

Organizers: Greg Voth, Scott Feller

	Sunday (June 9 th)	Monday (June 10 th)	Tuesday (June 11 th)	Wednesday (June 12 th)	Thursday (June 13 th)	Friday (June 14 th)
7:30 am - 9:00 am		Breakfast				
9:00 am - 9:30 am		Bill Wimley				Departure
9:30 am - 10:00 am		Ed Lyman				Departure
10:00 am - 10:30 am		Kalina Hristova				Departure
10:30 am - 11:00 am		Coffee Break				Departure
11:00 am - 11:30 am		Jessica Swanson				Departure
11:30 am - 12:00 pm		Alan Grossfield				Departure
12:00 pm - 12:30 pm		Lunch				Departure
12:30 pm - 1:00 pm		Lunch	Rachael Mansbach	Linda Columbus	Doug Tobias	
1:00 pm – 1:30 pm		Lunch	Greg Voth	Klaus Gawrisch	Helgi Ingolfsson	
1:30 pm – 2:00 pm		Jeffery Klauda	Sarah Veatch	Antoinette Killian	Roger Koeppe	
2:00 pm - 2:30 pm		J. C. Gumbart	Jaroslav Majewski	Alex Pak	Toby Allen	
2:30 pm - 3:00 pm		Ilya Levental	Coffee Break	J Kent Blasie	An Ghysels	
3:00 pm - 3:30 pm		Coffee Break	Joe Falke	Coffee Break	Coffe Break	
3:30 pm - 4:00 pm		Siewert-Jan Marrink	Stephanie Tristram-Nagle	Anne Kenworthy	Scott Feller	
4:00 pm - 4:30 pm		Frank Brown	Steve White	Denise Greathouse	Lukas Tamm	
4:30 pm - 5:00 pm		Angel Garcia	Rich Pastor	Juan Vanegas	Tamara Bidone	
5:00 pm - 5:30 pm	Informal Reception Penthouse RM 501 5-10 pm		John Nagle	Michael Brown	Randy Stockbridge	
5:30 pm - 6:00 pm	RM 501		Gerald Feigenson			
6:00 pm - 7:00 pm	RM 501		Happy Hour			
7:00 pm - 7:30 pm	RM 501		Banquet Dinner			
7:30 pm - 8:00 pm	RM 501		Banquet Dinner			
8:30 pm - 9:00 pm	RM 501		Banquet Dinner			
9:00 pm - 9:30 pm			Banquet Dinner			
9:30 pm - 10:00 pm			Banquet Dinner			
Number of Talks: 40		11	10	9	9	

Biological Membranes and Membrane Proteins Schedule

Sunday, June 9th, 2019

5:00pm-10:00 pm: Informal Reception and Cash Bar, Inn at Loretto Penthouse, RM 501

Monday, June 10th, 2019

7:30am – 9:00am: Breakfast

9:00am – 9:30am: Wimley, Bill
Synthetic Molecular Evolution of Hemocompatible Antimicrobial Peptides

9:30am – 10:00am: Lyman, Ed
Shear Viscosity and Dynamic Response of All-Atom and Coarse-Grained Simulation Models

10:00am – 10:30am: Hristova, Kalina
Mechanism of Action of Peptides That Cause PH-Triggered Macromolecular Poration of Bilayers

10:30am - 11:00am: Coffee Break

11:00am – 11:30am: Swanson, Jessica
Amphiphile-Membrane Translocation from the Lens of CG and Atomistic Simulations

11:30am – 12:00pm: Grossfield, Alan
Understanding Membrane Composition Effects on Antimicrobial Lipopeptide Aggregation Using Molecular Simulation

12:00pm – 1:30pm: Lunch Break

1:30pm – 2:00pm: Klauda, Jeffrey
Modeling the Stratum Corneum Lipid Matrix and Plasmalogen Lipids for Neuronal Membranes

2:00pm – 2:30pm: Gumbart, J.C.
Distribution of Mechanical Stress in the Escherichia Coli Cell Envelope

2:30pm – 3:00pm: Levental, Ilya
The Lipidomic and Biophysical Asymmetry of a Mammalian Plasma Membrane

3:00pm – 3:30pm: Coffee Break

3:30pm – 4:00pm: Marrink, Siewert-Jan
Computational Modeling of Realistic Cell Membranes

4:00pm – 4:30pm: Brown, Frank
Determination of membrane elastic constants from simulations

4:30pm – 5:00pm: Garcia, Angel
Uncovering the dynamics of a Molecular Switch: Atomistic Simulations of the interaction of KRas with membranes

Tuesday, June 11th, 2019

12:30pm – 1:00pm: Mansbach, Rachael (LANL)
Membranes and Machine Learning

1:00pm – 1:30pm: Voth, Greg
New Insights from the Multiscale Computer Simulation of Membrane Targeting and Remodeling Processes

1:30pm – 2:00pm: Veatch, Sarah
Beyond Protein Organization: Some Thoughts on Other Ways That Membranes With Domains Can Be Useful

2:00pm – 2:30pm: Majewski, Jaroslaw
Shiga Toxin Binding Induces Lipid Condensation: A Mechanism for Generating Membrane Curvature. X-ray scattering studies

2:30pm – 3:00pm: Coffee Break

3:00pm – 3:30pm: Falke, Joe
Regulation of Master Kinases on Membrane Surfaces in the PIP3 Signaling Pathway

3:30pm – 4:00pm: Tristram-Nagle, Stephanie
Elastic and Structural Results of the Antimicrobial Peptides WLBU2 and D8 Interacting with Membranes

4:00pm – 4:30pm: White, Steve
Membrane protein assembly via the SecA ATPase

4:30pm – 5:00pm: Pastor, Rich
Simulation of Membrane Permeability, and the Need for Polarizable Force Fields

5:00pm – 5:30pm: Nagle, John

A Potpourri of Results for Simple Lipid Bilayers: Component Volumes, DPPC Gel Phase Structure, Poisson Ratio, Tilt Modulus Criticality

5:30pm – 6:00pm: Feigenson, Gerald
Ld/Lo line tension calculated from pairwise lipid interaction energies

6:00 – 7:00pm: Happy Hour/Cash Bar

7:00 – 10:00pm: Banquet Dinner

Wednesday, June 12th, 2019

12:30pm – 1:00pm: Columbus, Linda
Physical Properties of Membranes and Membrane Mimics: Potential Impact on Membrane Protein Structure

1:00pm – 1:30pm: Gawrisch, Klaus
Structural Studies on Cannabinoid Receptor Type II, CB2

1:30pm – 2:00pm: Killian, Antoinette
Solubilisation of Membranes into Nanodiscs by Styrene-Maleic Acid Copolymers: Insights from Model Membrane Studies

2:00pm – 2:30pm: Pak, Alex
A Multiscale Framework to Include Solvent Effects in Implicit-Solvent Coarse-Grained Lipid Models

2:30pm – 3:00pm: Blasie, J Kent
Comparison of Different Models for the Voltage-Dependent States of Kv-Channels with the Time-Resolved Neutron Interferometry Data for KvAP

3:00pm – 3:30pm: Coffee Break

3:30pm – 4:00pm: Kenworthy, Anne
High Throughout Analysis of Membrane Phase Behavior

4:00pm – 4:30pm: Greathouse, Denise
Is Fraying Important for Transmembrane Helices?

4:30pm – 5:00pm: Vanegas, Juan
Feeling the Force: Understanding Mechanosensation Through Local Stress Calculations and Steered Simulations"

5:00pm – 5:30pm: Brown, Michael
Life and Death of Proteins Exposed to Extreme X-Ray Photons

Thursday, June 13th, 2019

12:30pm – 1:00pm: Tobias, Doug
Anomalous Subdiffusion of a Large Protein in the Plasma Membrane

1:00pm – 1:30pm: Ingolfsson, Helgi
Simulation Campaign Linking Macro and Micro Scale Using Machine Learning Reveals
RAS Membrane Dynamics

1:30pm – 2:00pm: Koeppe, Roger
Arginine Exit, Helix Distortion and a 310 Helix at a Membrane Surface

2:00pm – 2:30pm: Allen, Toby
Simulations to Understand Lipid Variations in the Dipole Potential

2:30pm – 3:00pm: Ghysels, An
Modeling Techniques for Oxygen and Water Permeability Through Membranes

3:00pm – 3:30pm: Coffee Break

3:30pm – 4:00pm: Feller, Scott
Configurational Entropy of Polyunsaturated Lipids

4:00pm – 4:30pm: Tamm, Lukas
The Role of Cholesterol and Lipid Rafts in Virus Infection

4:30pm – 5:00pm: Bidone, Tamara
Multiscale model of cell adhesions assembly from transmembrane integrins

5:00pm – 5:30pm: Stockbridge, Randy
Structural Sodium Ions in Membrane Protein Assembly