

Physical Chemistry of Biomembranes

Organizers: Atanu Acharya and Chayan Dutta

March 23-26, 2026

Monday PM

Georgia World Congress Center | B216

A. Acharya, C. Dutta, *Organizers* | J. Gumbart, *Presiding*

2:00 PM. Introduction.

2:10 PM. Transient protein structure guides surface diffusion pathways for electron transport in membrane supercomplexes. **A. Singharoy**

2:40 PM. Enabling atomistic modeling and simulation of complex lipid structures and cellular membranes with xMAS Builder. N. Trebesch, **E. Tajkhorshid**

3:10 PM. Self reproducing lipid membranes. **N.K. Devaraj**

3:40 PM. Intermission.

3:50 PM. Lipid composition modulates structure, thermal stability and function of Membrane Proteins in Nanodiscs. **A. Das**, R. Das, T. Tang

4:20 PM. Design of functional membrane proteins through engineered dynamic hydrogen bonding networks. N.P. Jacob, V.T. Silverman, G. Prida Ajo, **H.T. Kratochvil**

4:50 PM. Intermission.

5:00 PM. Preorganized electric fields in voltage-gated sodium channels. **V. Vaissier Welborn**

5:30 PM. Influence of membrane on b-cell receptor activation. **S. Gnanakaran**

Physical Chemistry of Biomembranes

Organizers: Atanu Acharya and Chayan Dutta

March 23-26, 2026

Tuesday AM

Georgia World Congress Center | B5 - EXHIBIT HALL ChemPod 12

A. Acharya, C. Dutta, *Organizers* | C. Dutta, *Presiding*

8:00 AM. Protein import across and insertion into mitochondrial membranes. **J. Gumbart**

8:30 AM. Understanding lipid-receptor interactions enables new insights into GPCR pharmacology. **M. Eddy**

9:00 AM. Small-molecule permeation and condensate-membrane interactions probed by molecular simulations. Y. Qi, **Y. Wang**

9:30 AM. Intermission.

9:40 AM. Quantifying T cell receptor mechanics at membrane junctions using DNA origami tension sensors. **K. Salaita**

10:10 AM. Membrane-mediated assembly of tight junction claudin proteins. **S. Nangia**

10:40 AM. Intermission.

10:50 AM. GM1-mediated confinement of plastic nanoparticles on a GM1/POPC membrane: A single-molecule study. **D. Sil**, S.C. Mandal, A. Acharya, C. Dutta

11:10 AM. Martini 3 as a transferable force field: Applications to diverse bacterial lipopolysaccharides. **G. Gutishvili**, D.L. Lynch, J. Gumbart

11:30 AM. Atomistic modeling of bio-nano hybrids with iron oxide nanoparticles and the outer membrane of *Shewanella*. **T. Wei**

Physical Chemistry of Biomembranes

Organizers: Atanu Acharya and Chayan Dutta

March 23-26, 2026

Wednesday AM

Georgia World Congress Center | C209

A. Acharya, C. Dutta, *Organizers* | R. J. Vazquez, *Presiding*

8:00 AM. Interaction between biomolecular condensates and lipid membrane: Mechanistic insights from multi-scale analyses. **Q. Cui**

8:30 AM. New advances in understanding functionally diverse antibiotic permeability barriers in bacteria. **H. Zgurskaya**, I. Leus, J. Adamiak, C. Bergen, V. Rybenkov

9:00 AM. Role of Native Environments in Biochemical Charge Transfer Network. **A Acharya**

9:30 AM. Intermission.

9:40 AM. A tale of two tails: Membrane response to environmental conditions through isomerization. S. Raza, **J.V. Vermaas**

10:10 AM. Unbiased simulation of proton-coupled passive diffusion of ionizable drugs through the membrane. J. Clayton, **J. Shen**

10:40 AM. Intermission.

10:50 AM. Cytochrome P450 2u1 determines the local metabolic fate and antitumor activity of Thymus Tumor-Targeting drugs. **Y. Li**, T.Y. Tang, P. Chapman, A. Das, E. Tajkhorshid

11:10 AM. Effect of GM1 ganglioside on the model membrane-nanoplastic interaction. **S.C. Mandal**, D. Sil, C. Dutta, A. Acharya

11:30 AM. Photoswitchable interlocked molecules for modulating membrane structure and memristive behavior. **V. Garcia-Lopez**, U. Conthagamage, R. Rajeshwar, P. Podar, M. Smith, J. Smith, C.P. Collier

Physical Chemistry of Biomembranes

Organizers: Atanu Acharya and Chayan Dutta

March 23-26, 2026

Wednesday PM

Georgia World Congress Center | A302

A. Acharya, C. Dutta, *Organizers* | A. Gahlmann, *Presiding*

2:00 PM. Processive pointed-end polymerization turns actin treadmilling on its head.

S. Shekhar

2:30 PM. Lipid composition actively reshapes the folding pathway of a membrane-inserting peptide. **C. Baiz**

3:00 PM. Illuminating membrane disruption with single vesicle spectroscopy. **S. Quinn**

3:30 PM. Intermission.

3:40 PM. Interrogating membrane biophysics with time-resolved fluorescence spectroscopy and microscopy. **R.J. Vazquez**

4:10 PM. Cell-free protein biosensing of the activity of hard-to-reach organelle ion channels. **S. Daniel**

4:40 PM. Intermission.

4:50 PM. Unraveling plastic-induced denaturation of model peptides: Single-molecule FRET insights. **G. Tripathi**, S. Nguyen

5:10 PM. Molecular foundation models for predicting self-assembly and phase separation in aqueous mixtures. **H. Liu**, C. Ekosso, A. Glagovich, S.E. Maurer, J. Schrier

5:30 PM. Computational tools in mechanobiology: Exploring the mechanostability of extracellular proteins. **R.C. Bernardi**

Physical Chemistry of Biomembranes

Organizers: Atanu Acharya and Chayan Dutta

March 23-26, 2026

Thursday AM

Georgia World Congress Center | B309

C. Dutta, *Organizer* | A. Acharya, *Organizer, Presiding*

8:00 AM. Nanoscale Interactions of Plastic Nanoparticles on Biomembranes Using Single Particle Imaging. **C. Dutta**

8:30 AM. μ -Bots as self-transporting carriers and mechanodrugs. **S. RAKSHIT**

9:00 AM. Measuring the bound times of transient protein complexes in living cells using 3D single-molecule imaging and membrane tethering. R. Casper, I. Grewal, **A. Gahlmann**

9:30 AM. Intermission.

9:40 AM. Impact of cyclodextrins on lipid asymmetry, membrane structure, and flip-flop. P. Hymas, **J.C. Conboy**

10:10 AM. Exploring the impact of the cell wall on bacterial membrane behavior using second harmonic scattering. **T.R. Calhoun**

10:40 AM. Intermission.

10:50 AM. pH-dependent structure and dynamics of lipid nanoparticles: Insights from 2D IR spectroscopy and MD simulations. **X. Chen**, C. Xu, C. Baiz

11:10 AM. Investigating the properties of PRM:SH3 Interactions using artificial intelligence and molecular dynamics. **S. Kim**

11:30 AM. Molecular insights on perturbation of nanoplastics on biomembranes from neutron scattering. **S. Qian**, H. Zhang, W. Leite, A.E. Whitten, P.A. Zolnierczuk, Y. Yuan, Q. Zhang

Special thanks to our sponsors for their generous support:

