# **Research Topics:**

# Glycopolymer Biophysics

Large linear glycopolymers known as glycosaminoglycans (GAGs) coat living cells in the form of a glycocalyx that binds to charged cations and biological macromolecules.

### · Biomolecular Condensates

Cationic polyelectrolytes such as nucleic acids, glycopolymers and many proteins can form assemblies with cationic protein domains to form 2-phase solutions and many biological functions are controlled using structures.

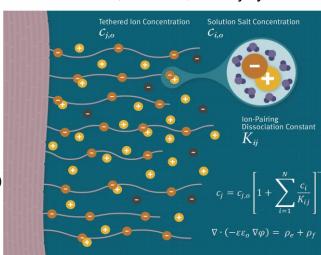
# · Biomolecular Simulation and Modeling

All-atom and coarse-grained molecular dynamic (MD) simulations are used to elucidate structure-function relationships. Mean field models known as Born-modified Poisson Nernst Planck are used to elucidate MD observations

#### **Current Work:**

Application of Multivalent Innate Immune Signaling Target (MIIST) glycopolymers for managing autoimmunity through control of vascular inflammation, infection, and injury.

A Continuum Model of Mucosa with Glycan-lon Pairing. James D. Sterling and Shenda M. Baker Macromolecular Theory and Simulations, Volume 27, Issue 2, March 2018. (Cover Image)



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### **Selected Publications:**

- Mathematical modeling of microscale biology: Ion pairing, spatially varying permittivity, and Born energy in glycosaminoglycan brushes; W. Ceely et al., Physical Review E., February 2023, 107:024416.
- Quantitative insights into electrostatics and structure of polymer brushes from microslit electrokinetic experiments and advanced modelling of interfacial electrohydrodynamics; R. Zimmermann et al., Current Opinion in Colloid & Interface Science 2022, 59:101590.
- The role of the cell surface glycocalyx in drug delivery to and through the endothelium; Lu Fu et al. Advanced Drug Delivery Reviews, 2022, 184, 114195.
- ➤ Ion pairing and dielectric decrement in glycosaminoglycan brushes; James D. Sterling, Wenjuan Jiang, Wesley Botello-Smith and Yun L. Luo, *Journal of Physical Chemistry B*, 2021, 125, 10, 2771-2780.



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