Theoretical Polymer and Soft Materials in the Wang Group

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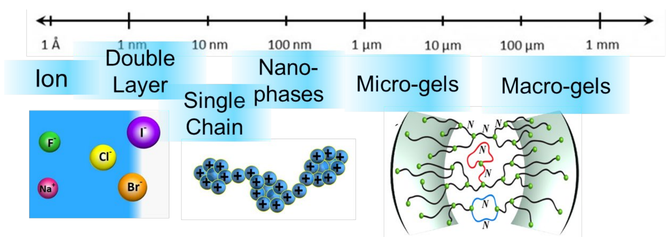
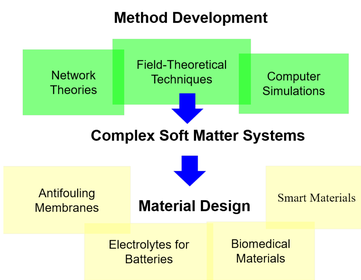
Wang Group Theme

Ions, Polymers, and Gels



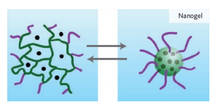


Challenges:

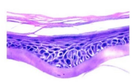
- Wide range of length scales
- Multiple components and interactions
- Inhomogeneous system with interfaces
- Retention of molecular information

Complex Polymer Networks: Towards the Design of Smart Materials

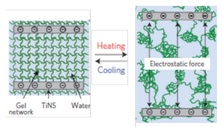
Motivation: Stimuli-responsive materials



Sensors

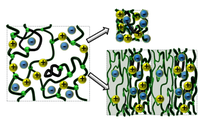


Artificial muscles



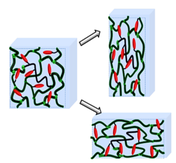
Soft Actuators

Ionic Gels

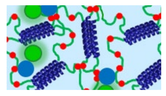


Complex phase behaviors

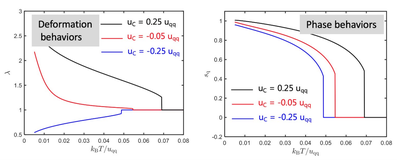
Liquid Crystal Elastomers



Biopolymer Networks

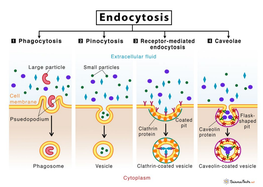


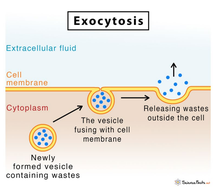
- Topology
- Elasticity
- Permittivity

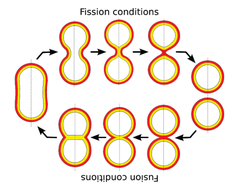


Polymer Interactions, Morphological Evolutions, and Micromechanics

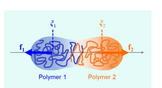
Motivation: Vesicle Fission and Fusion in Cells

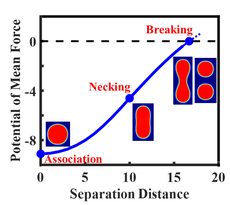




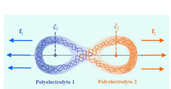


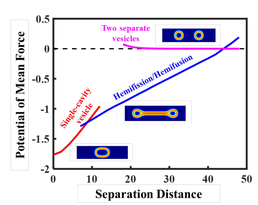
Neutral Polymers



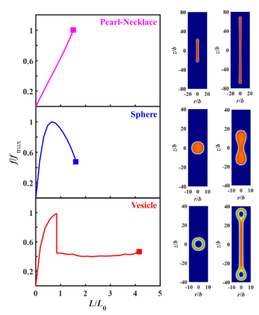


Polyelectrolyte Vesicles



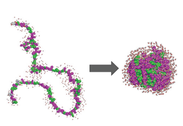


Micromechanics



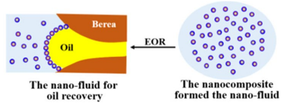
Structure and Dynamics of Polyelectrolytes

Motivation: Polyelectrolytes are everywhere



Protein Folding

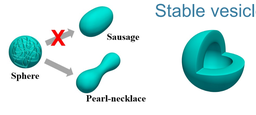
Protein Aggregation



Enhanced Oil Recovery

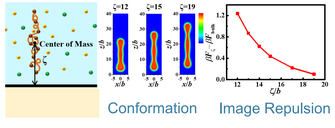
Method: A new field-based polymeric theory

Single-chain Conformation



Stable vesicle

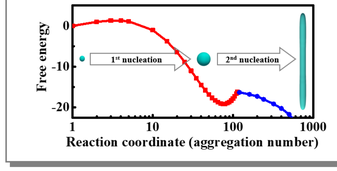
Interfacial Activity



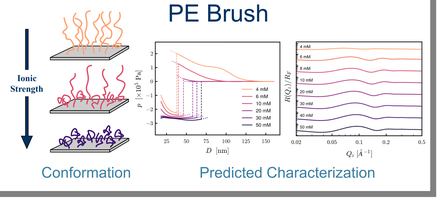
Conformation

Image Repulsion

Nucleation in PE Aggregation



PE Brush

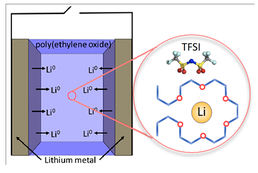


Conformation

Predicted Characterization

Ion Solvation and Transport in Polymer Electrolytes

Motivation: Rational Design of Polymer Electrolyte for Li Batteries

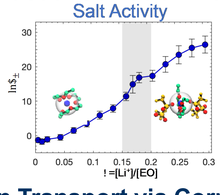


Objective:
Relating microscopic solvation structures to continuum electrolyte transport

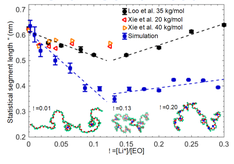
Method:
Computer simulations
Collaboration with experiments

Unusual Solvation Behavior

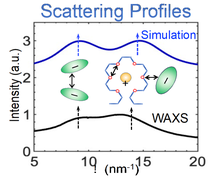
Salt Activity



Chain Conformation

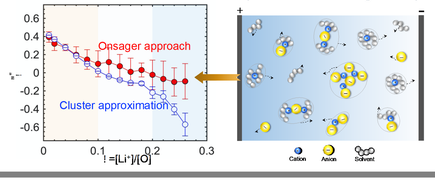


Scattering Profiles

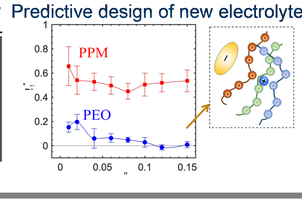


Ion Transport via Correlated Motion

Cation transference and dynamic heterogeneity



Predictive design of new electrolytes



Electrostatics at Interfaces of Membranes and Ion-Channels

Motivation: Membrane Fouling Driven by Electrostatics

A self-consistent theory to model double layers beyond the reach of PB theory:

Incompressibility variable

$$-\nabla\cdot[\epsilon(\boldsymbol{r})\nabla\psi(\boldsymbol{r})] = \rho_{ex}(\boldsymbol{r}) + \sum_{i=+,-} z_i \frac{e^{\mu_i}}{v_i}\exp[-z_i\psi(\boldsymbol{r}) - u_i(\boldsymbol{r}) - v_i\eta(\boldsymbol{r})]$$

Self energy of the ion:

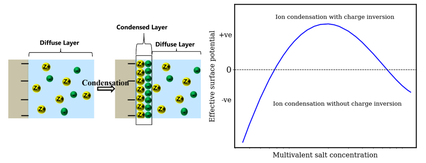
$$u_\pm(\boldsymbol{r}) = \frac{z_\pm^2}{2}\int d\boldsymbol{r}'d\boldsymbol{r}'' h_\pm(\boldsymbol{r}'-\boldsymbol{r})G(\boldsymbol{r}',\boldsymbol{r}'')h_\pm(\boldsymbol{r}''-\boldsymbol{r})$$

A new model to resolve the electrostatic correlation function at both the length scale of ion and interface

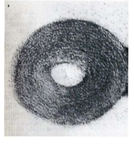
Analytical solution — Numerical calculation

$$G(\boldsymbol{r}',\boldsymbol{r}'') = G_{\text{short}}(\boldsymbol{r}',\boldsymbol{r}'') + G_{\text{long}}(\boldsymbol{r}',\boldsymbol{r}'')$$

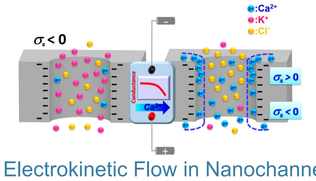
Electrostatic correlation induced ion condensation and charge inversion



Applications



Encapsulation of DNA in viruses



Electrokinetic Flow in Nanochannels

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