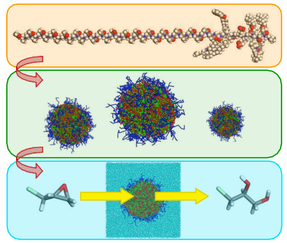
Computational NanoBio Technology Lab

Led by Professor Seung Soon Jang

Nanomaterials & Energy

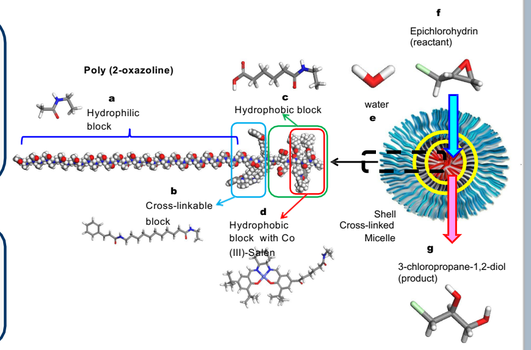
Multicompartment Micelle (MCM) Nanoreactor



MCMs for immobilized-catalysis nanoreactors
- Modeling and optimization of triblock copolymer structure
- Mesoscale simulation of MCM self-assembly
- Calculation of optimal cohesive energy
- Studies in reactant and product species diffusion/transport phenomena through micelle

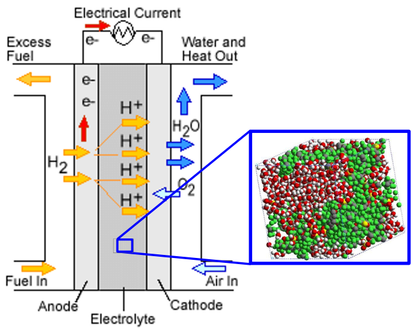
Mean square displacement and potential of mean force
Common measure of the spatial extent of random motion of targeted atoms to probe their diffusivity in the micelle

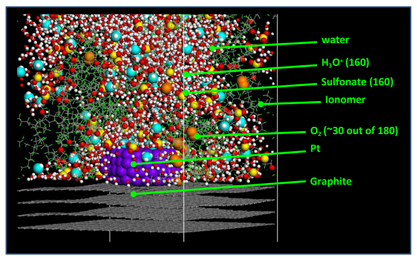
Limiting steps in the process
Diffusivity of reactant and product determine the limiting rate of the overall process

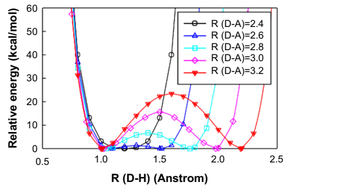


Polymer Electrolyte Membrane Fuel Cell (PEMFC)

Fuel cell technology
- Investigating the materials in the three-phase region of a PEMFC
- Platinum cluster stability and dissolution mechanism
- Electrolyte structure and transport properties
- Three-phase MD:
  - Catalyst coverage
  - O_2 transport
  - Interface structure







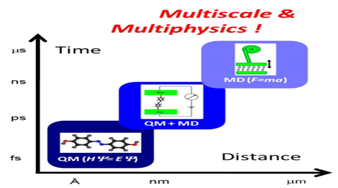
MD techniques can be used to probe energies of different donor-acceptor separation distances

Computational Tools

Molecular Dynamics
- Large simulation of materials system to obtain bulk physical properties and measure nanoscale features

Machine Learning
- To establish a mapping that would otherwise be difficult to obtain theoretically from a given data set.

Quantum Mechanics
- Electronic structure methods include density functional theory, MP perturbation theory and configuration interaction.



Electrochemical Energy Storage

Solid Polymer Electrolyte (SPE)

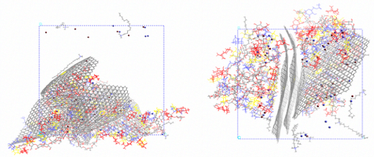
SPE for Li-ion batteries
- Discovery of new SPEs with moderate-high ionic conductivity at room temperature.
- Safer, non-corrosive, non-flammable, thermally stable, light-weight
- Molecular dynamics on Li diffusion in SPE.
- Analysis on ion conductivity

Overcome SPE issues
- Resistance increase at lower temperatures
- Weak chemical stability

Graphene Fiber Nanocomposite

Introduction:
- Graphene-based materials are being investigated for use in several applications such as batteries, super-capacitors, and fuel cells.

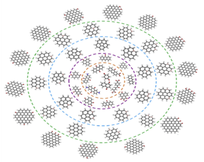
Goal:
- Find thermal and thermodynamic transitions that lead to the measured electrical conductivity jump in the graphene polymer nanocomposite fiber utilizing computational materials science methods namely molecular dynamics simulations

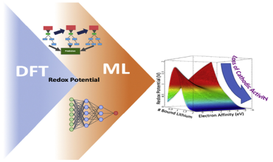


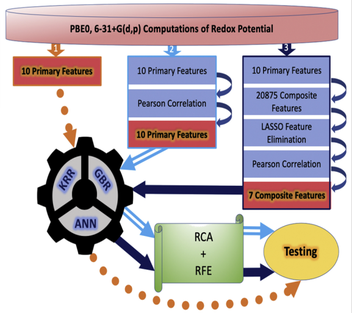
Graphene Polymer Nanocomposite Fiber models shown after undergoing equilibrium Molecular Dynamics (MD) simulations

Organic Electrode Discovery Machine Learning Approach

Goal
- Elucidate the relationship between molecular structure and Redox potential.
- Design/develop new organic electrodes for battery

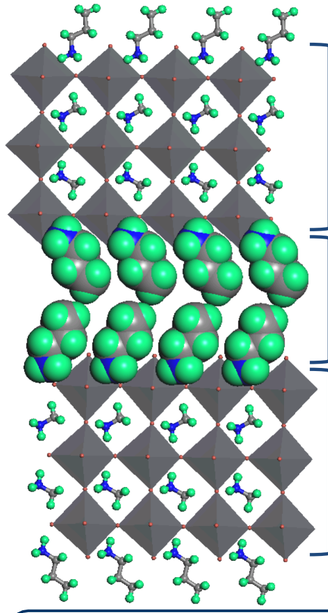






Perovskite Optoelectronics

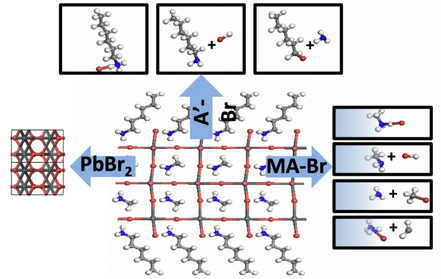
Hybrid Organic-Inorganic Perovskites (HOIP)



3D Perovskite
- ABX_3 perovskites show great promise for use in photovoltaics.
- Computational study of elemental and hybrid perovskites to determine band gap - composition relationship using DFT and machine learning.

2D Layered Perovskite
- $A_{n-1}A'_2B_nX_{3n+1}$ generally more stable than 3D perovskite phase.
- Exhibit high photoluminescence quantum efficiencies.
- Investigating means of band gap tuning of layered perovskites by adjusting layer size and composition.
- Comparing the role of aliphatic spacers with that of aromatic ones in HOIP's through DFT modeling.
- Modeling of layered perovskite for Li-ion battery application.

Machine Learning Study of Perovskites
- Utilizing artificial neural network approach to analyze the contribution that certain structural identifiers have on the band gap of 2D layered perovskites and 3D perovskite oxides.
- Screening for perovskites with optimal band gap for photovoltaic performance



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