Computational NanoBio Technology Lab

Led by Professor Seung Soon Jang

Georgia Tech

CNBT Lab. Since 2002

Nanomaterials & Energy

Multicompartment Micelle (MCM) Nanoreactor

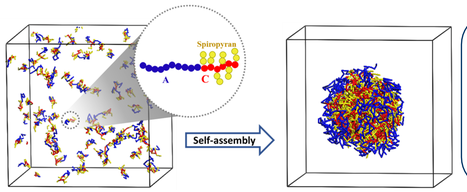
Flory-Huggins χ −Parameter

- Miscibility between polymer and polymer/solvent
- Connolly volume, dielectric constant, solvation free energy

$$\Delta E_{ij}^{mix} = \frac{1}{2n}(V_{ref})\left[\frac{E_{ij}^{*}}{V_{ij}}\left(\frac{Z_{ij}}{n_i}+\frac{Z_{ji}}{n_j}\right)-\left(\frac{E_{ii}^{*}Z_{ii}}{V_{ii}\,n_i}+\frac{E_{ii}^{*}Z_{ii}}{V_{jj}\,n_j}\right)\right]+\frac{E_{solv,i\,in\,j}^{*}}{V_{ij}}$$

Ionic Species

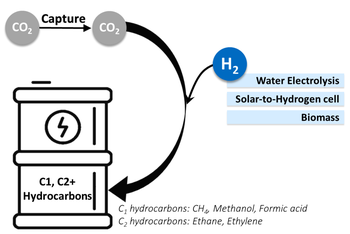
$$\chi = \frac{\Delta E_{ij}^{mix}}{RT}$$



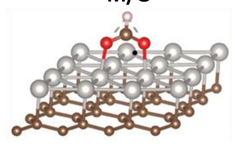
- Mesoscale simulation of self-assembly MCMs in water
- Effect of size and ratio of MCMs on morphology
- Structural analysis via radial distribution function calculation

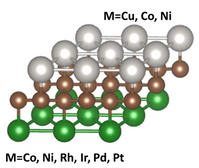
Metal/graphene (M/G) 2D Hybrid Electrocatalyst for CO_2 Reduction to HCOOH

Hydrogen Storage



M/G



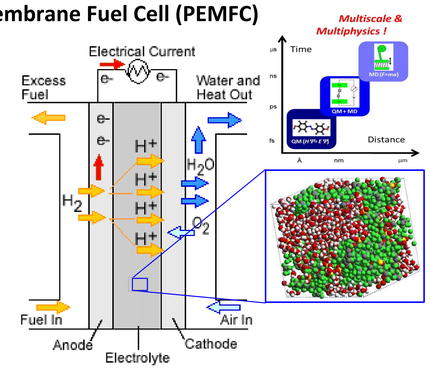


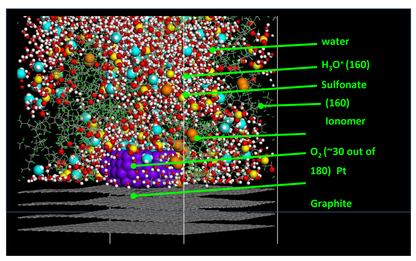
- Metal/graphene carries unique electronic structures
- Hybridized graphene in M/G allows deposition of additional metal layer.
- Onset potential of CO_2RR and HER was evaluated

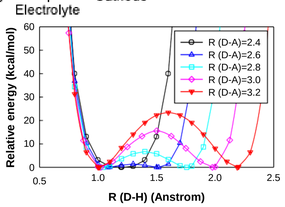
Polymer Electrolyte Membrane Fuel Cell (PEMFC)

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
Simulate bulk physical properties and measure nanoscale features.

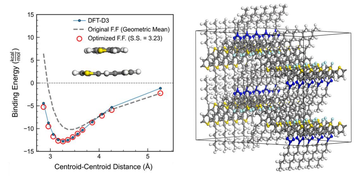
Quantum Mechanics
Density functional theory, MP perturbation theory and configuration interaction.

Machine Learning
Efficient and predictive surrogate models for materials properties, screening and selection.

Applied Materials Design and Discovery

Semiconducting Polymers

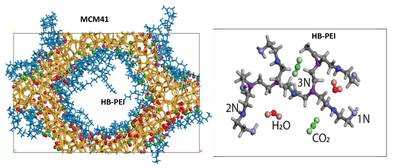
Within our multiscale modeling framework, incorporating DFT, MD, and ML, we investigate the intricate ordering competition between backbones and sidechains, unraveling their influence on morphological and thermal transitions of SCPs.



Direct Air Capture (DAC)

Innovative sorbents for CO_2 capturing
Using the DFT and MD simulation approach, we aim to find novel materials for carbon capture.

- Composite of hyperbranched Polyethylene Imine and MCM-41.
- Effect of moisture on adsorption efficiency
- Transport and diffusion of carbon dioxide



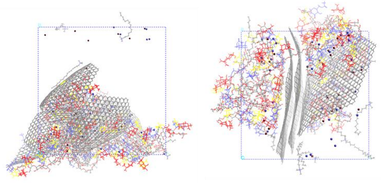
Microwave-induced Heating

Microwave-driven selective heating process are investigated with molecular dynamics simulations.

- Water-polyethylene oxide mixed system
- Activated molecular rotation
- Selective dielectric heating
- Intensity and frequency dependency

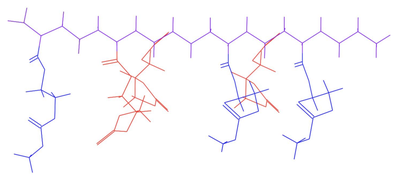
Graphene Fiber Nanocomposite

Graphene-based materials are being investigated for use in several applications such as batteries, super-capacitors, and fuel cells to find thermal and thermodynamic transitions that lead to the measured electrical conductivity jump in the graphene polymer nanocomposite fiber.

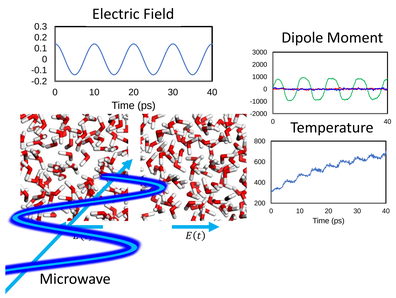


Solid Polymer Electrolytes (SPE)

Molecular dynamics simulations are used to model novel carbonate-based polymers to enhance Li-ion battery stability.

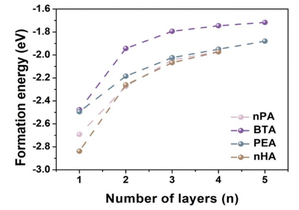


EC/DMC Copolymer



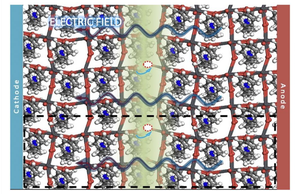
Energy Storage and Conversion

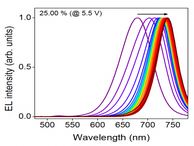
Spacer Steric Effect on Band Gap



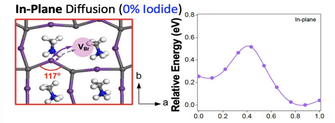
Hybrid Organic-Inorganic Perovskites (HOIP)

- Class of self-assembled quantum-well structures with excellent optoelectronic properties.
- Blue luminescence efficiency is still low.
- Spectral instability is a significant impediment to their exploitation for commercial LEDs.
- DFT calculations for the fine-tuning of the emission wavelength by **adjusting the organic spacer** and **mixing halide composition**.

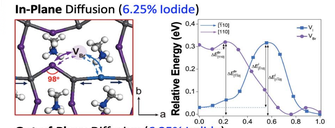




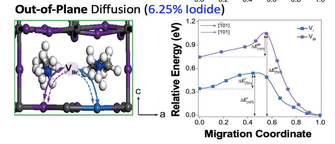
In-Plane Diffusion (0% Iodide)



In-Plane Diffusion (6.25% Iodide)



Out-of-Plane Diffusion (6.25% Iodide)

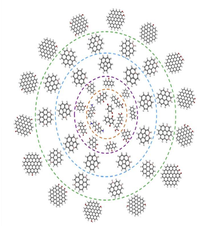


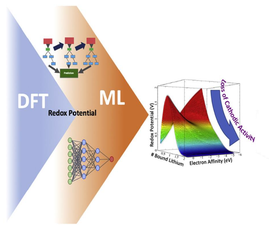
Spectral Instability in Mixed Halide HOIP

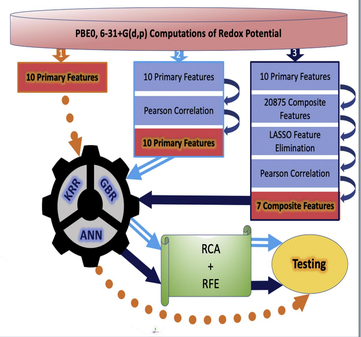
- NEB calculations reveal source of spectral instability: Br^- is kinetically limited due to steric effects from neighboring I^-.
- Thus, Br^-/I^- domains will be formed under bias.

Organic Electrode Discovery Machine Learning Approach

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







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