**Nanomaterials & Energy**

**Multicompartiment Micelle (MCM) Nanoreactor**
- Flory-Huggins $x$ - Parameter
- Miscibility between polymer and polymer/solvent
- Connolly volume, dielectric constant, solvation free energy

**Metal/graphene (M/G) 2D Hybrid Electrocatayst for CO₂ Reduction to HCOOH**
- Metal/graphene carries unique electronic structures
- Hybridized graphene in M/G allows deposition of additional metal layer
- Onset potential of CO₂ RR and HER was evaluated

**Hydrogen Storage**
- Capture-Hydrogen-Solar-to-Hydrogen-cell

**Polymer Electrolyte Membrane Fuel Cell (PEMFC)**
- 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
  - O₂ transport
  - Interface structure

**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

**Energy Storage and Conversion**

**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

**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 SCs

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

**Spacer Steric Effect on Band Gap**
- Elucidate the relationship between molecular structure and Redox potential
- Design/develop new organic electrodes for battery

**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

**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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