Surface Studies and Laser Spectroscopy with Geri Richmond and Friends

A brief presentation by Brandon Schabes
Air/Water Studies: Modeling Behavior at Aerosol Interfaces

How do soluble organics orient at the surface?
- Aerosol aging
- Surface chemistry
- Gas-phase pollutant uptake and absorption
- pH dependence

SO₂ Uptake: Acid Rain Climate Change

How do salts affect gas uptake?

How do organics and salts affect uptake?
**Oil-water studies: Model for a variety of molecular processes.**

**Polypelectrolytes**
- Proteins: Cellular adsorption
- Humic acids: Water remediation
- Flooding & flocculent: oil recovery

**Surface Modified Nanoparticles**
- Nanoparticle self-assembly & emulsion stabilization
- Water remediation
- Targeted drug delivery

**What factors affect polyelectrolyte adsorption to an oil/water interface?**
- Molecular weight?
- Charge Density?
- Specific isomer?
- Solution pH?
- Metal ions?

**Monomer unit**

**Under what conditions do polyelectrolyte and surfactant modified nanoparticles adsorb to and orient at an oil/water interface?**
Goal: Fabricate and analyze semiconductor material combinations that will promote impact ionization at heterojunctions.

More efficient heterojunction solar cells

Impact ionization increases quantum efficiency!

Molecular dynamics corroborate air/water spectra

- Combination of classical dynamics and density functional theory
- Predicts minutiae of molecular orientation at interface
- Generates vibrational sum frequency spectra
  - Compare with experimental spectra
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Experimental Techniques

Sum frequency spectroscopy: Vibrational spectra of interfacial molecules.

Air/water studies

\[ \omega_{\text{SF}} = \omega_{\text{IR}} + \omega_{\text{VIS}} \]

Oil/water studies

Scattering technique: curved surfaces

Pump-probe experiment for solar cell research

Molecular Dynamics Simulations

Other techniques: FTIR, interfacial tension, dynamic light scattering

Simulations of interfaces are performed to generate computational descriptions of experimental observations.