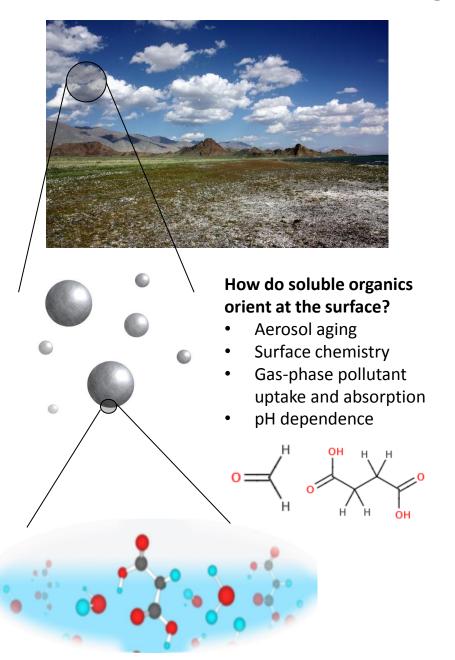
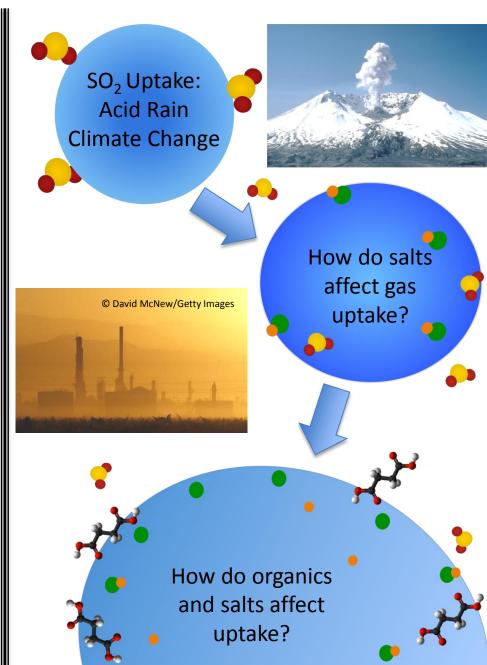


## Air/Water Studies: Modeling Behavior at Aerosol Interfaces

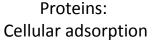




## Oil-water studies: Model for a variety of molecular processes.

#### Polyelectrolytes





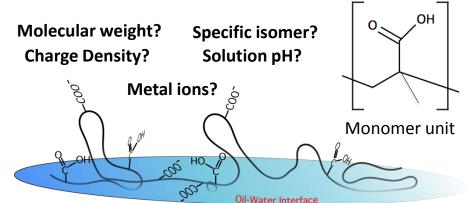


Humic acids: Water remediation



Flooding & flocculent: oil recovery

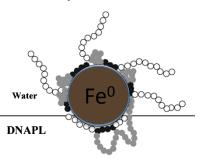
What factors affect polyelectrolyte adsorption to an oil/water interface?



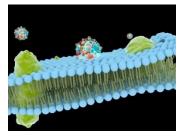
#### **Surface Modified Nanoparticles**



Nanoparticle self-assembly & emulsion stabilization

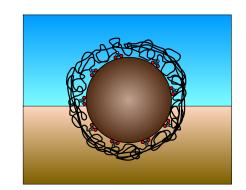


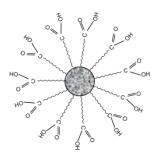
Water remediation



Targeted drug delivery

Under what conditions do polyelectrolyte and surfactant modified nanoparticles adsorb to and orient at an oil/water interface?

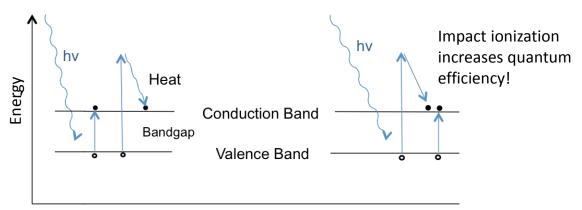


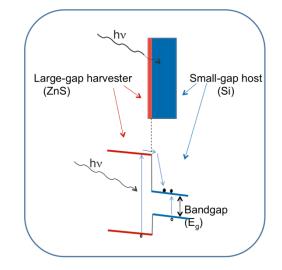


### More efficient heterojunction solar cells

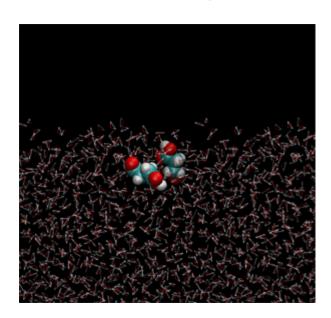
Goal: Fabricate and analyze semiconductor material combinations that will promote impact

ionization at heterojunctions.





# Molecular dynamics corroborate air/water spectra

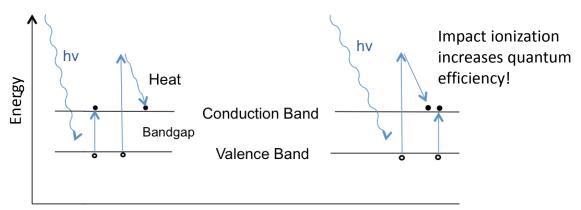


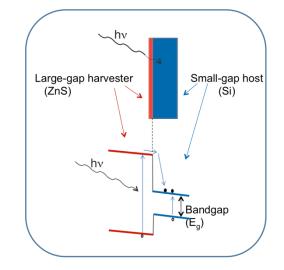
- Combination of classical dynamics and density functional theory
- Predicts minutiae of molecular orientation at interface
- Generates vibrational sum frequency spectra
  - Compare with experimental spectra

### More efficient heterojunction solar cells

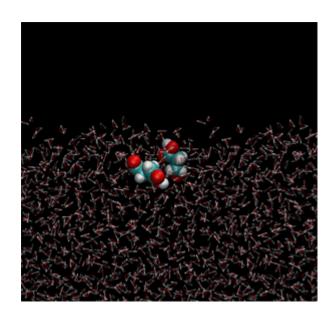
Goal: Fabricate and analyze semiconductor material combinations that will promote impact

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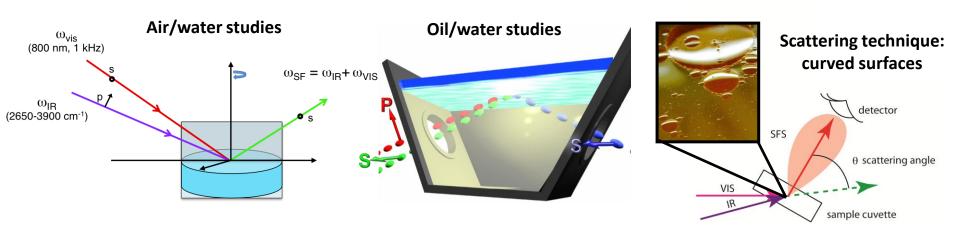
## Molecular dynamics corroborate air/water spectra



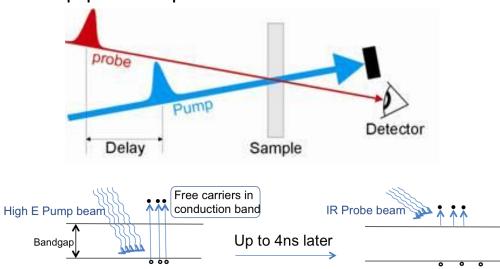
- Combination of classical dynamics and density functional theory
- Predicts minutiae of molecular orientation at interface
- Generates vibrational sum frequency spectra
  - Compare with experimental spectra

#### **Experimental Techniques**

Sum frequency spectroscopy: Vibrational spectra of interfacial molecules.

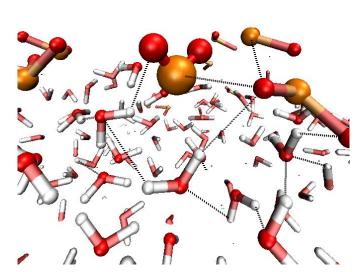


Pump-probe experiment for solar cell research



Other techniques: FTIR, interfacial tension, dynamic light scattering

**Molecular Dynamics Simulations** 



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



Pat Blower



Dr. Katy Plath



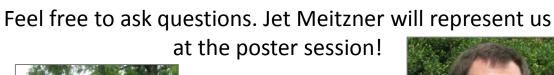
Ellen Robertson



Dr. Fred Moore



Dr. Stephanie Ota





**Brock Tillotson** 



Dr. Nick Valley



**Brandon Schabes** 



Dr. Jennifer Hensel



Laura McWilliams