

**Molecular modelling of water adsorption on  
hydrophobic and hydrophilic  
self-assembled monolayers as proxies for  
atmospheric organic surfaces**

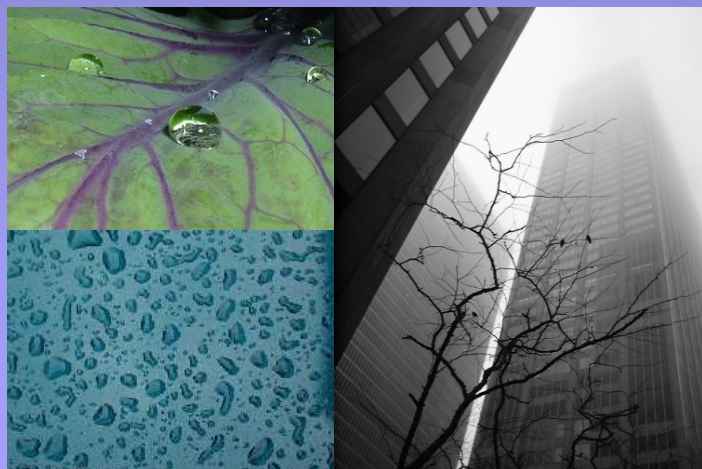
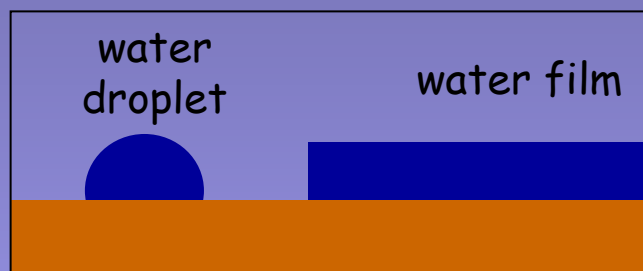
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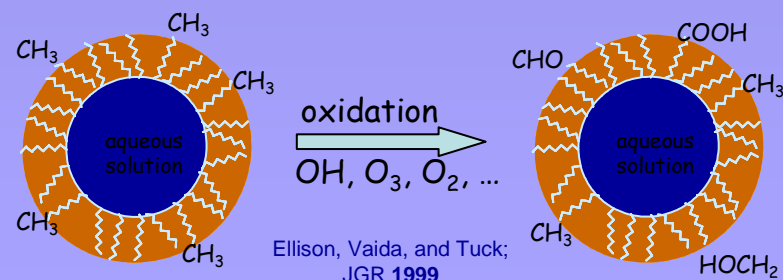
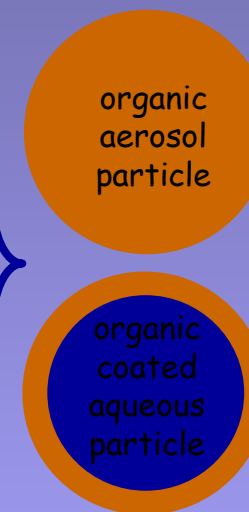
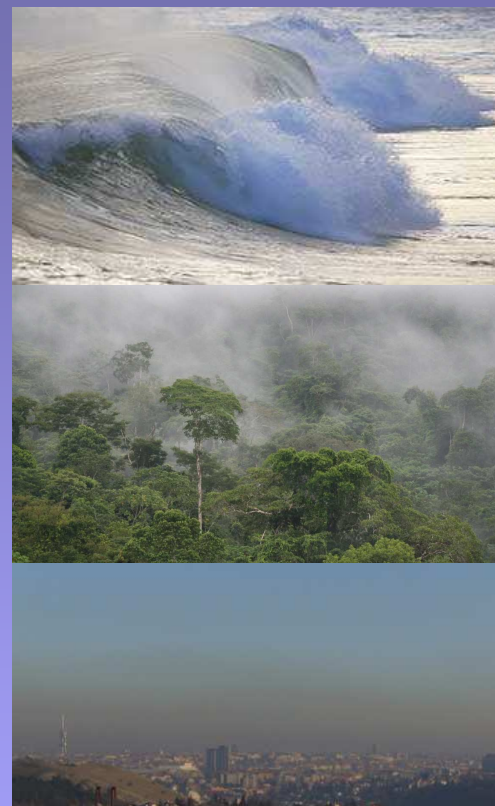
**POSTER # 26**

# Motivation

## a) Water uptake on atmospheric surfaces



## b) Water uptake on atmospheric organic aerosols



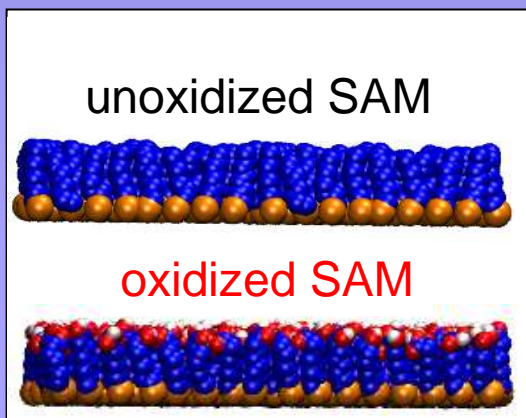
Ellison, Vaida, and Tuck;  
JGR 1999

## Questions

- What is the uptake of water on **hydrophobic** organic surfaces?
- How does it differ from uptake by **hydrophilic** organic surfaces?
- What effect does **surface roughness** have on water uptake?
- How does water interact with organic surfaces of **mixed** hydrophobic and hydrophilic character?
- How does the hydrophilic and hydrophobic **domain size** affect the water binding on these surfaces?

## Methodology

- Mixed hydrophobic/hydrophilic **self-assembled monolayers** of alkanethiols on gold used as models of organic coatings on atmospheric aerosols



1. **Molecular dynamics simulations (Prague)**
2. **Experiments (University of California Irvine)**
  - Temperature programmed desorption (Hemminger group)
  - Attenuated total reflection FTIR spectroscopy (Finlayson-Pitts group)

Hydrophobic SAM

Hydrophilic SAM

