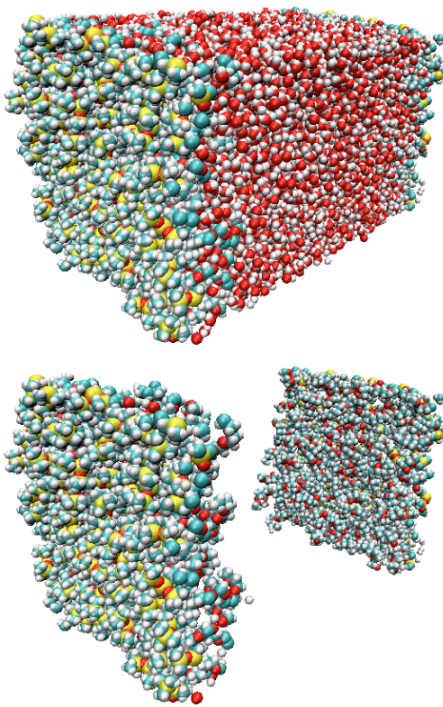


Bachelor's/ Master's thesis:  
**Simulation of Superspreaders at air/water and  
polymer/water interfaces**

**Topic:** Trisiloxane surfactants are widely used in paints, cosmetics, and pesticides because of their unique capability as "superspreaders," facilitating the ultra-rapid spreading of aqueous solutions on hydrophobic substrates. Because trisiloxanes are both chemically unstable and toxic, there has been a large effort in the last 20 years to uncover the effects that promote superspreading. Despite numerous studies, the driving mechanisms have not yet been identified.



A central problem in the research on superspreading is that experiments cannot observe the molecular-scale behavior of the surfactants. In this project, you will study the unique physical properties and behavior of trisiloxane surfactants at interfaces using Molecular Dynamics (MD) simulations, a simulation method of steadily increasing importance in academia and industry. Your work will include various aspects of MD, including

preparation of the simulations, their execution on high performance computers, and their analysis.

**Requirements:** You should have a background in chemical engineering, material science, simulation sciences, natural sciences, or a related area, and a general interest in simulation science and chemistry. Basic programming skills in any language (preferably Python) are required.