

# Substrate Preparation for Ultrafast Vibrational Spectroscopy Experiments

**CNF Project Number: 1936-10**

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*Primary Source(s) of Research Funding: National Science Foundation*

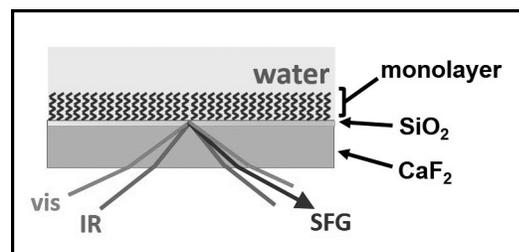
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*Primary CNF Tools Used: Oxford ALD FlexAL*

## Abstract:

Water is ubiquitous and an active component in many natural and technological processes. Vibrational spectroscopy can be used to probe the structure and dynamics of water in a variety of environments. We use sum-frequency generation, a surface specific vibrational spectroscopy, to probe the structure and dynamics of interfacial water at chemically tunable surfaces. Interfaces with tunable surface character are created with self-assembled monolayers. In order to create substrates compatible for both silane self-assembly and sum-frequency generation, infrared and visible transparent  $\text{CaF}_2$  windows are coated with  $\text{SiO}_2$ . Then after surface functionalization with silane monolayers, the water structure and dynamics at the interfaces can be explored with sum-frequency generation.



## Summary of Research:

Water is an active component in many natural and technological processes [1]. Interfaces terminate the H-bonded network of water. We aim to study the structure and dynamics of water at self-assembled monolayers (SAMs) with varying surface character using sum-frequency generation (SFG) spectroscopy. In SFG, an infrared photon interacts with a dipole transition of the molecule and a visible photon excites the molecule to a virtual electronic state where it can undergo an anti-Stokes Raman transition resulting in a photon at the sum of the two incident frequencies being emitted [2,3].

In order to collect SFG spectra of solid-aqueous interfaces, we must probe through the window so the infrared photons are not absorbed by water. However, silica, a common SAMs substrate, also absorbs in the infrared. To create an infrared and visible transparent substrate compatible with SAMs syntheses, we start with a calcium fluoride ( $\text{CaF}_2$ ) window, which is transparent through the visible and infrared. Then approximately 10 nm of  $\text{SiO}_2$  is deposited on the  $\text{CaF}_2$  window via atomic layer deposition (ALD) with the Oxford ALD FlexAL. The  $\text{SiO}_2$  layer is thin enough to not absorb all the IR photons and prevent SFG spectra of the sample from being collected, but thick enough to form a surface compatible with the self-assembly of silanes.

Once the  $\text{SiO}_2$  is deposited, hydrophobic, hydrophilic, or mixed monolayers are synthesized with self-assembly of silanes on the surface. Figure 1 shows a schematic of the surface in contact with water. Then, the surfaces and water at the surfaces are analyzed with SFG [2-6].

## References:

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