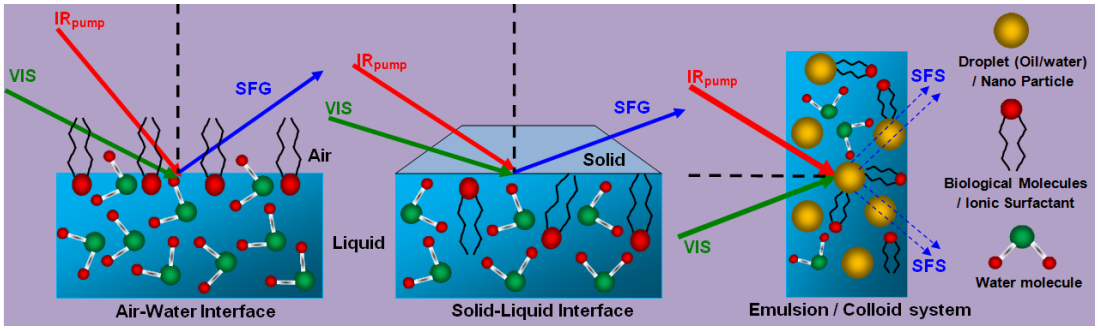
Sum frequency generation vibrational spectroscopy

Sum frequency generation (SFG) vibrational spectroscopy is a surface active and molecular specific technique. It is emerging as a widely recognized non-linear optical spectroscopic tool for studying the conformation and orientation of various adsorbed molecules at various interfaces. SFG spectroscopy carries the ability to provide the vibrational spectrum of the chemical moieties present at the interfaces. It is a second order nonlinear optical process where two pulsed laser beams, one of fixed visible frequency and the other of tunable (broadband) infrared frequency are overlapped spatially and temporally at an interface to generate SFG signal. The frequency of the generated SFG signal is the sum of the two incident field frequencies. By measuring the SFG signal as a function of the infrared frequency, a vibrational spectrum of the species at the interfacial region can be obtained. Figure 1 shows a schematic representation of the SFG principle with the model sample systems.



The intensity of the output SFG signal is proportional to the absolute square of the surface response coefficient ($\chi_s^{(2)}$) which is a combination of nonresonat and resonant combination of each vibrational mode and is given by,

$$I_{SFG} \propto \left|\chi_s^{(2)}\right|^2 = \left|\chi_{NR}^{(2)} + \chi_R^{(2)}\right|^2 = \left|\chi_{NR}^{(2)} + \sum_q \frac{A_q}{\omega_{IR} - \omega_q + i\Gamma_q}\right|^2$$

here, $\chi_{NR}^{(2)}$ and $\chi_R^{(2)}$ are from nonresonant and resonant contribution. A_q, ω_q and Γ_q are the strength, resonant frequency and damping coefficient of the q^{th} vibrational mode, respectively.

Key issues to be addressed:

- What are the conformational changes of the biological macromolecules/drugs/surfactants upon adsorption on planar / miniature droplet surfaces?

- Impact of the charged groups of the biological macromolecules / surfactants on hydrogen bonding environment and the conformation of polar interfacial water molecules.

- How are the conformations of the biological macromolecules going to behave upon the introduction of electrolytes and other biological guest molecules?