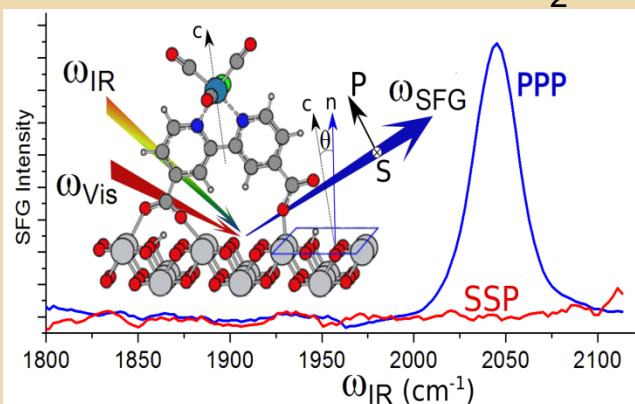


Covalent Attachment of a Rhenium Bipyridyl CO₂-Reduction Catalyst to Rutile TiO₂ Probed by SFG

Tianquan Lian, Department of Chemistry, Emory University, Atlanta, GA 30322

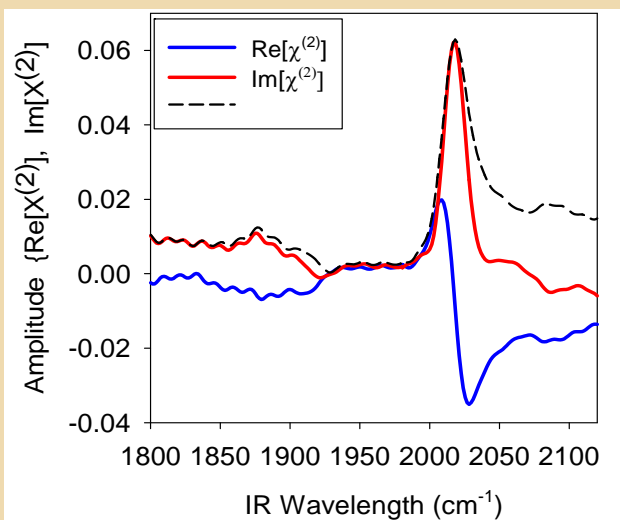
SFG spectra and a computed structure of ReC0A on TiO₂



➤ Vibration Sum Frequency Generation (SFG) spectroscopy is a surface selective and *in situ* technique for recording vibration spectra of adsorbates at interfaces relevant to solar energy conversion, such as in solar cells and in photoelectrochemical cells.

➤ The binding geometry of ReC0A (a model CO₂ reduction catalyst) on the Rutile TiO₂ (001) surface has been determined by a combined SFG measurement and computational modeling study.

Heterodyne detected SFG Spectra:



➤ heterodyne detection of SFG signal allows a) the measurement of sub-monolayer of molecules on a semiconductor surface – important for identifying catalytic intermediates; b) improvement of signal-to-noise ratio and reduce data averaging time – essential for using SFG to probe interfacial dynamics in a pump/probe experiment; and c) the determination of both the real and imaginary part of the second order susceptibility – simplifying spectral assignment.