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Small Molecules and Sum Frequency Generation Probes of Nanoparticulate TiO_2

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Anatase TiO_2 is known to photo catalytically mineralize a wide variety of pollutants and pathogens, both airborne and in aqueous solution. One of the major benefits of basing water treatment systems on TiO_2 is that it is environmentally benign and so non toxic that it is used as a colorant in creamy salad dressing. The primary impediment to wide spread implementation of a TiO_2 based system for water decontamination is that the quantum efficiency in contact with condense phase water is less than 5%. Since the quantum efficiency for destruction of airborne materials is greater than 80%, the potential for increased efficiency is very real. To convert the potential to practice, the oxidation mechanism needs to be more fully understood. We will report on the results of using a nonlinear optical spectroscopy, sum frequency generation (SFG) as an *in situ* probe of interactions at the TiO_2 surface. Results suggest that the dominant oxidation mechanism converts from a direct to an indirect mechanism as the water content (vapor pressure) increases. This presentation will discuss the probe technique as well as the results.