NSF Award in Engineering

Principal investigator: Franz Geiger, chemistry, Weinberg College of Arts and Sciences

- Project: Olefins at the Surfaces of Transparent Oxides Studied With Coherent Vibrational Spectroscopy
- Start Date: September 1, 2009
- Total Award Amount: $300,000

How the results of this project will benefit society:
Reactions of inorganic and organic species on metals and metal oxides have received much attention in heterogeneous catalysis, culminating in the 2007 Nobel Prize in chemistry. The scientific community, especially scientists working on heterogeneous catalysis, will benefit from improved molecular-level information regarding the structure and orientation of olefins and related catalytically relevant molecules. The spectroscopic and structural data from this work will allow other scientists in the field to refine chemical and mechanistic models for describing catalytically important heterogeneous processes at solid/gas interfaces, obtain molecular-level information on the molecular orientation of organic compounds at oxide surfaces, benchmark their spectroscopic and structural data from theory calculations, and improve the accuracy in predicting catalytic activity. By directly and indirectly interacting with students and policy makers, the PI’s integrated research, education, and public outreach activities will continue to be powerful tools for communicating scientific efforts to the general public.

The problem the project is trying to solve:
This research expands the fundamental molecular-level understanding of heterogeneous catalysis. It will also enable advances of existing theoretical and mechanistic frameworks for interfacial phenomena found in nature. Motivated by the lack of thoroughly assigned vibrational spectra for most catalytically relevant hydrocarbons adsorbed to oxide surfaces, the PI extends the pioneering surface spectroscopy experiments on hydrocarbons of others from metal surfaces towards oxide surfaces.

How this project will work:
This research focuses on laboratory measurements aimed at elucidating the molecular orientation of catalytically relevant hydrocarbons at oxide surfaces. The PI will determine the molecular orientation and distributions of common saturated and unsaturated chiral and achiral hydrocarbons relevant to heterogeneous catalysis (C2 through C6 derivatives as well as quinuclidine derivatives) on SiO2, Al2O3, and related oxides by assigning their vibrational surface spectra using vibrational sum frequency generation in the CH stretching region. He will develop a vibrational mode assignment strategy for determining the symmetry of a given vibrational mode from SFG spectra, allowing them to identify whether a given mode is symmetric or asymmetric. This strategy will greatly facilitate the analysis of the vibrational spectra and molecular orientation and structure determination of catalytically relevant hydrocarbon species at catalytically relevant oxides.

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