



KYOTO UNIVERSITY
Global COE Program

INTEGRATED
MATERIALS SCIENCE

Global COE Special Lectures

Recent Advances in Spectroscopy and Surface Science

An interdisciplinary forum on spectroscopy, physical chemistry, surface science, and biophysical chemistry offers researchers and students from different scientific disciplines the opportunity to attend three lectures and participate in discussions.

Organizer: Shigeichi Kumazaki

Date and Time: November 17, 2010 13:25 – 17:00

Place: Seminar House, Graduate School of Science, Kyoto University

Registration: No formal registration and fees are required. Please inform of your attendance by e-mail to the organizer ([kumazaki\[at\]kuchem.kyoto-u.ac.jp](mailto:kumazaki[at]kuchem.kyoto-u.ac.jp)).
Please replace [at] with @.

Program

13:25 – 13:30 Opening remarks

13:30 – 14:40

"Imaging the Femtosecond Time Scale Correlated Electron-Nuclear Dynamics in Surface Photodesorption"

Prof. Hrvoje Petek

Department of Physics and Astronomy, University of Pittsburgh

We employ time-resolved two-photon photoemission to characterize electronic structure and photoinduced dynamics of chemisorbed alkali atoms on noble metal surfaces. Photoinduced charge transfer excitation of the lowest energy sigma resonance of Cs on Cu or Ag surfaces turns on repulsive forces between atom and surface initiating nuclear wave packet motion on a dissociative potential energy surface. Energy, momentum, and time resolved measurements of photoemission from desorbing atoms provide information on the nuclear wave packet motion and the concomitant changes in the surface electronic structure. In particular, we use time-dependent momentum imaging of photoemission from the excited state to explore the correlation between the electron and nuclear motions.

14:40 – 14:50 Break

14:50 – 16:00

“Amyloid Fiber Formation and Inhibition Studied with 2D IR Spectroscopy”

Prof. Martin Zanni

Department of Chemistry, University of Wisconsin

Among the tools available to structural biologists, 2D IR spectroscopy has a unique combination of structure and time-resolution. With this technique, it is possible to probe structural changes with bond-specificity and femtosecond accuracy. This talk will present recent results on applying the technique to study the aggregation of the amyloid polypeptide implicated in type 2 diabetes. In conjunction with isotope labeling, transient 2D IR spectra have been collected that reveals a detailed pathway of the peptide backbone as it forms toxic oligomers and fibrils. Moreover, we have studied the action of a peptide inhibitor, and learned that it prevents fiber formation by binding to one of the two beta-sheets, which occurs about half-way along the aggregation pathway. Together, the fiber growth and drug inhibition mechanisms are two of the most detailed structural studies performed so far on this toxic polypeptide.

16:00 – 16:10 Break

16:10 – 16:50

“Hydrogen-Bond Engineering and Proton Dynamics in Real Space”

Prof. Hiroshi Okuyama

Department of Chemistry, Graduate School of Science, Kyoto University

Proton-relay reactions in a model hydrogen-bond system were induced and observed using a scanning tunneling microscope (STM). We assembled hydrogen-bonded "wires" consisting of a single water molecule and two or three hydroxyl groups on Cu(110) at low temperatures with the STM. Using these model systems, proton-relay reactions along the hydrogen-bond wires, i.e., $\text{H}_2\text{O}-\text{OH}-\text{OH}(-\text{OH}) \rightarrow (\text{OH}-)\text{OH}-\text{OH}-\text{H}_2\text{O}$, were studied in real space. The reactions are triggered by vibrational excitations of the molecular adsorbates by the tunneling electrons followed by sequential interconversions of covalent and hydrogen bonds, resulting in the "structural transfer" of a water molecule. The experimental findings are rationalized by ab initio calculations for adsorption geometry, active vibrational modes, and reaction pathway, in order to reach a detailed microscopic picture of the elementary processes.

16:50 – Closing remarks

Notes: No beverages are served at the Seminar House.

For further information, please contact Shigeichi Kumazaki,

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