

FINAL PROGRAM

SEVENTEENTH ANNUAL SYMPOSIUM

LABORATORY FOR SURFACE MODIFICATION

<http://www.physics.rutgers.edu/lsm/>

Thursday, February 27, 2003

9:00 a.m. to 5:00 p.m.

Rutgers, The State University of New Jersey



**Fiber Optics Auditorium
Busch Campus
Piscataway, New Jersey**

Final Program

SEVENTEENTH ANNUAL SYMPOSIUM LABORATORY FOR SURFACE MODIFICATION

8:15 Registration, coffee

8:45 Introductory Remarks

**Professor Theodore E. Madey, Director of Laboratory for Surface Modification
Professor Holly Smith, Dean, Faculty of Arts and Sciences**

I. Nanoscale Phenomena

**Chairperson, Professor Charles Glashauser,
Acting Chair, Department of Physics and Astronomy**

**9:00 Quantum Size Effects and CO Adsorption at Cu(100) Surfaces, A. G. Danese,
and R. A. Bartynski, *Dept. of Physics and Astronomy.***

**9:15 Faceting Induced by Adsorption of Oxygen on Re(12 $\bar{3}$ 1), H. Wang¹, W. Chen¹,
A. S. Y. Chan¹, J. E. Rowe², and Theodore E. Madey¹, ¹*Dept. of Physics and Astronomy,*
²*North Carolina State University.***

**9:30 Structure and Electrical Characterization of Organic Monolayers on Au,
W.Jiang¹, N. Zhitenev², B. de Boer², M. Frank¹, D. Abusch-Magder², S. Yang², A.
Ermakov¹, O. Celik, Z. Bao², Y.Chabal³ and E. Garfunkel¹, ¹*Dept. of Chemistry,* ²*Bell
Labs, Lucent Technologies,* ³*Dept. of Biomedical Engineering.***

**9:45 TEM investigation of Carbon Iron-Fluoride Nanocomposites, F. Cosandey, F.
Badway, N. Pereira, and G. G. Amatucci, *Dept. of Ceramic and Materials Engineering.***

**10:00 Selective Growth of ZnO Nanotips on Various Substrates by MOCVD, H. H.
Chen, S. Muthukumar, J. Zhong, J. Hu, Y. Lu, *Dept. of Electrical and Computer
Engineering.***

10:15 First-principles Study of Oxygen Vacancy Pinning of Domain Walls in PbTiO₃,
L. He and D. Vanderbilt, *Dept. of Physics and Astronomy.*

10:30 -Coffee Break and Poster Session-

II. Biomaterials and Condensed Films

Chairperson, Professor Kathryn Uhrich
Department of Chemistry and Chemical Biology

11:00 Highlight presentation - The Importance of Surface Chemistry in Understanding Cell-Material Interactions, Joachim Kohn, *Dept. of Chemistry.*

11:30 Mechanochemical Stimulation of the Synthesis of Hydroxyapatite from Nonionic Surfactant Emulsions, C. -W. Chen¹, R. E. Riman¹, K. Brown², K. S. TenHuisen², and V. F. Janas², ¹*Department of Ceramic and Materials Engineering,* ²*Johnson & Johnson Corporate Biomaterials Center.*

11:45 Oxygen Plasma Treatment of Poly(dimethylsiloxane) Stamps, B. Langowski and K. Uhrich, *Dept. of Chemistry.*

12:00 Dynamics of Electron-induced Decomposition of CF₂Cl₂ and CCl₄ Co-Adsorbed with Water (Ice), N. S. Faradzhev¹, C. C. Perry², D. O. Kusmierik¹, D. H. Fairbrother², and T. E. Madey¹, ¹*Department of Physics and Astronomy,* ²*Johns Hopkins University.*

12:15 - 1:45

-Lunch and Poster Session-

POSTER PAPERS

- 1. Development of Ultrafast Near Field Optical Microscopy**, S. Lou, F. Zimmermann, R. Bartynski, *Dept. of Physics and Astronomy*.
- 2. Adsorption and Decomposition of Acetylene on Clean and Oxygen-covered Ir(210)**, W. Chen¹, I. Ermanoski¹ and T. E. Madey¹, H. H. Hwu² and J. G. Chen², ¹*Dept. of Physics and Astronomy*, ²*University of Delaware*.
- 3. Structural, Electronic and Catalytic Properties of Clean and Overlayer-Covered Ir(210)**, I. Ermanoski¹, W. Chen¹, M. J. Gladys¹, J. S. Quinton¹, T. E. Madey¹, M. Ulrich², and J. E. Rowe², ¹*Dept. of Physics and Astronomy*, ²*North Carolina State University*.
- 4. Electron- and Photon-stimulated Desorption of Alkali and Alkaline-earth Atoms from a Lunar Basalt Surface and a Model Mineral Surface**, B. V. Yakshinskiy and T. E. Madey, *Dept. of Physics and Astronomy*.
- 5. TPD and STM Studies of Chlorosilane Desorption Mechanisms from Cl-exposed Cu/Si(111) Surfaces**, D. V. Potapenko, S. E. Sysoev, A. V. Ermakov, D. Maithil, and B. J. Hinch, *Dept. of Chemistry*.
- 6. Nanometer Scale Thin Film Structure Analysis Using MeV He Ion Beams**, L. S. Wielunski, *Dept. of Physics and Astronomy*.
- 7. Thermal Properties of Cerium Oxides as Potential High-k Dielectrics**, R. Barnes¹, T. Nishimura², T. Gustafsson¹, E. Garfunkel³, ¹*Dept. of Physics and Astronomy*, ²*AIST, Tsukuba, Japan*, ³*Dept. of Chemistry*.
- 8. Structural Characteristics of Mg_xZn_{1-x}O Films Grown on R-plane Sapphire Substrates**, G. Saraf, S. Muthukumar, J. Zhong, Y. Chen, Y. Lu, *Dept. of Electrical and Computer Engineering*.
- 9. Wet Chemical Etching of ZnO Films Grown on R-Sapphire**, J. Zhu, N. W. Emanetoglu, Y. Chen, Y. Lu, *Dept. of Electrical and Computer Engineering*.
- 10. SAW Characteristics in Piezoelectric Materials Modified by ZnO Nanotips**, Z. Zhang, W. Pan, S. Muthukumar, Y. Chen, Y. Lu, *Dept. of Electrical and Computer Engineering*.
- 11. Bulk Acoustic Wave Characteristics in Piezoelectric Mg_xZn_{1-x}O Films**, R. H. Wittstruck¹, X. Tong¹, N. W. Emanetoglu¹, J. Zhu¹, Y. Lu¹, A. Ballato², ¹*Dept. of Electrical and Computer Engineering*, ²*U. S. Army Communications-Electronics Command, Fort Monmouth*.
- 12. Channel Mobility Study of 4H-SiC Lateral JFET**, P. Sannuti, X. Li, F. Yan, K. Sheng, J. H. Zhao, *Dept. of Electrical and Computer Engineering*.
- 13. Understanding Response in TDDFT**, F. Zhang, N. T. Maitra, K. Burke and R. J. Cave, *Dept. of Chemistry*.
- 14. A Model Description of Surface Second Harmonic Generation at Hydrogen Covered Si(001) Surface**, M. B. Yilmaz, A. Rajagopal, F. Zimmermann, *Dept. of Physics and Astronomy*.

15. **The Local Density Approximation Can Yield Accurate Excitations to Rydberg States**, A. Wasserman, N.T. Maitra, and K. Burke, *Dept. of Chemistry*.
16. **Nano-crack Growth by Ar⁺ Implantation with H⁺ Plasma Processing for SOI Exfoliation**, B. Chen, A.Y. Usenko, W. N Carr, *NJIT*.
17. **Unoccupied Electronic States of Ag/Al(100)**, J. F. Veyan^{1,2}, P. Häberle², W. Ibañez², R. Bartynski³, ¹*Departamento de Física, Universidad Católica, Valparaiso, Chile*, ²*Departamento de Física, Universidad Técnica, Valparaiso, Chile*, ³*Department of Physics and Astronomy*.
18. **Comparative Study of Bioactive Bone Cement surfaces by SEM and NSOM**, R. Vargas-Coronado¹, J. V. Cauich-Rodríguez¹, L. F. Garfias² ¹*Centro de Investigación Científica de Yucatán A.C, Mérida, Yucatán, México*, ²*Lucent Technologies*.

III. Semiconductor Surfaces and Interfaces

Chairperson, Professor David G. Daut
Department of Electrical and Computer Engineering

- 1:45 Highlight presentation - Exploring the Limits of Transistor Scaling with Electron Microscopy**, David Muller, *Bell Labs, Lucent Technologies.*
- 2:15 Nucleation, Growth, and Structure of Alternative Gate Oxides**, M. M. Frank^{1,4}, S. Dörmann², M.-T. Ho², Y. J. Chabal^{1,2,3}, S. Sayan¹, E. Garfunkel¹, G. D. Wilk⁴, and M. L. Green^{4,5}, ¹*Dept. of Chemistry*, ²*Dept. of Physics and Astronomy*, ³*Dept. of Biomedical Engineering*, ⁴*Agere Systems*, ⁵*IMEC, Belgium.*
- 2:30 Band Alignment Issues of High-K Gate Stack Structures**, S. Sayan¹, R.A. Bartynski², M. Croft², T. Emge¹ and E. Garfunkel¹, ¹*Dept. of Chemistry*, ²*Dept. of Physics and Astronomy.*
- 2:45 Nanochemistry of H, O₂ and H₂O at 3C-SiC Surfaces**, F. Amy¹, Y. Chabal², ¹*Princeton University*, ²*Dept. of Chemistry and Dept. of Biomedical Engineering.*
- 3:00 -Coffee Break-**

IV. Surfaces and Interfaces Theory and Applications

Chairperson, Professor Lisa Klein,
Ceramic and Materials Engineering

- 3:30 Tailoring of SAW Properties of ZnO-based Multilayer Structures**, Y. Chen, K. Wu, N. W. Emanetoglu, Y. Lu, *Dept. of Electrical and Computer Engineering.*
- 3:45 Revisiting Ni Growth on W(111): Faceting, Thermal Stability, and Reactivity**, Q. Wu^{1,2}, J. Kolodziej³, H. Wang^{1,2}, and T. E. Madey¹, ¹*Dept. of Physics and Astronomy*, ²*Dept. of Chemistry*, ³*Instytut Fizyk, Jagellonian University, Poland.*
- 4:00 Electronic Polarization at Surfaces and in Thin Films of Organic Molecular Crystals (OMC)**, E. Tsiper¹, Z. G. Soos², ¹*Dept. of Chemistry*, ²*Princeton University.*
- 4:15 Growth and Thermal Evolution of Surface Structure in Ternary Sn-Si-Cu(001) Films**, L. V. Goncharova^{1,2}, A. V. Ermakov¹, D. V. Potapenko¹, B. J. Hinch¹, X.

Zhang³, D. R. Strongin³, ¹*Dept. of Chemistry*, ²*Dept. of Physics and Astronomy*, ³*Temple University*.

4:30

-End of Presentations/Talks; Laboratory Visits-

Abstracts for Talks

9:00 Quantum Size Effects and CO Adsorption at Cu(100) Surfaces, A. G. Danese, and R. A. Bartynski, *Dept. of Physics and Astronomy*.

Using direct and inverse photoemission (IPE) along with temperature programmed desorption (TPD) we have studied the effect of metallic quantum well (MQW) states on the adsorption of CO on the Cu/fccFe/Cu(100) system. The CO desorption temperature varies as a function of Cu overlayer thickness and is correlated with Cu MQW states passing through the Fermi energy. The results suggest that it is possible to modify chemisorption behavior at surfaces using quantum size effects. The possible mechanism for this effect will be discussed.

9:15 Faceting Induced by Adsorption of Oxygen on Re(12 $\bar{3}$ 1), H. Wang¹, W. Chen¹, A. S. Y. Chan¹, J. E. Rowe², and Theodore E. Madey¹, ¹*Dept. of Physics and Astronomy*, ²*North Carolina State University*.

Adsorption of oxygen on atomically-rough Re(1 2 -3 1) has been studied by means of low energy electron diffraction (LEED), Auger electron spectroscopy (AES) and high resolution soft X-ray photoemission spectroscopy (HRSXPS) using synchrotron radiation. The LEED results show that oxygen does not form any superstructure on the Re(1 2 -3 1) surface at room temperature. However, when the oxygen-covered surface is annealed to 700K, it is no longer planar and nanometer scale facets start to grow. From HRSXPS, new features associated with the facets can also be identified in the Re4f peaks. When the annealing temperature is 900K or higher, the surface is fully faceted. The lowest coverage of oxygen required for the complete faceting is about 0.5 monolayer. Unlike the bcc(111) or fcc(210) metal cases, the Re facets do not form three-sided pyramids. Instead, a ridge-like morphology is observed. The facet orientations of the ridge have been identified as (0 1 -1 0) and (1 1 -2 1), which is consistent with the field emission microscopy (FEM) results from our collaborators and kinematical simulations of the LEED patterns.

9:30 Structure and Electrical Characterization of Organic Monolayers on Au, W. Jiang¹, N. Zhitenev², B. de Boer², M. Frank¹, D. Abusch-Magder², S. Yang², A. Ermakov¹, O. Celik, Z. Bao², Y. Chabal^{1,3} and E. Garfunkel¹, ¹*Dept. of Chemistry*, ²*Bell Labs, Lucent Technologies*, ³*Dept. of Biomedical Engineering*.

STM, conductive tip AFM, and FTIR have been used to examine structural and electrical properties of organic monolayers for potential molecular electronics applications. Systems consisting of pure and mixed alkane-, thiophene- and phenyl-thiols were examined. Top electrode contacts were realized using vacuum evaporation, electroless deposition, stamp imprinting, gold nanoparticles, and direct tip-organic contact.

9:45 TEM investigation of Carbon Iron-Fluoride Nanocomposites, F. Cosandey, F. Badway, N. Pereira, and G. G. Amatucci, *Dept. of Ceramic and Materials Engineering*.

The microstructure and electrochemistry of FeF₃:C based carbon metal fluoride nanocomposites (CMFNCs) used as positive electrodes in Li-Ion batteries was investigated from 4.5 to 1.5V. The microstructure determined by combined electron diffraction, HRTEM and EELS revealed nanodomains of FeF₃ on the order of 1-20 nm encompassed in a matrix of carbon. Experimental data reveal a reversible metal fluoride conversion process with approximately one-third of the capacity involving a reduction reaction of Fe³⁺ to Fe²⁺. The remainder of the specific capacity occurred in a two-phase conversion reaction at 2V resulting in the formation of a finer Fe:LiF nanocomposite.

10:00 Selective Growth of ZnO Nanotips on Various Substrates by MOCVD, H. H. Chen, S. Muthukumar, J. Zhong, J. Hu, Y. Lu, Dept. of Electrical and Computer Engineering.

ZnO is a wide band gap semiconductor (E_g=3.32eV). ZnO nanotips have many interest properties as a result of very high exciton binding energy (~60meV) and the size effect. We report the selective growth of ZnO nanotips on various substrates by MOCVD. The ZnO nanotips are about 40nm in width, single crystalline and possess good optical property. These nanotips have potential applications in field emission devices and UV optoelectronic devices.

10:15 First-principles Study of Oxygen Vacancy Pinning of Domain Walls in PbTiO₃, L. He and D. Vanderbilt, Dept. of Physics and Astronomy.

Certain models of fatigue (i.e., the degradation of the saturation polarization with repeated switching) involve pinning of ferroelectric domain walls by point defects. However, the microscopic interactions between domain walls and point defects remain poorly understood. As a first step in this direction, we have investigated the interaction of oxygen vacancies and 180° domain walls in tetragonal PbTiO₃ using density-functional theory. Our calculations indicate that the vacancies do have a lower formation energy in the domain wall than in the bulk, thereby confirming the tendency of these defects to migrate to, and pin, the domain walls. The pinning energies are reported for each of the three possible orientations of the original Ti-O-Ti bonds, and attempts to model the results with simple continuum models are discussed.

11:00 Highlight presentation - The Importance of Surface Chemistry in Understanding Cell-Material Interactions, Joachim Kohn, Dept. of Chemistry.

When materials with clean surfaces are first introduced into biological fluids, proteins present in those biological fluids adsorb to the material surface. This seminal event is then followed by the attachment of cells to the material surface. Consequently, cells never interact with a material surface directly, but rather interact with the protein layer whose composition and conformation is dependent on the underlying material surface. The presence of the protein layer as an "adhesive interface" between the material and cells has made it extremely difficult to establish correlations between specific surface properties and the biological responses of cells and tissues. In this presentation, some of the surface science techniques used to study interfacial phenomena at the cell-material interface will be described. In addition, the challenges of both surface scientists and

biologists in understanding cell-material interactions will be discussed using several recent research projects as illustrative examples.

11:30 Mechanochemical Stimulation of the Synthesis of Hydroxyapatite from Nonionic Surfactant Emulsions, C. -W. Chen¹, R. E. Riman¹, K. Brown², K. S. TenHuisen², and V. F. Janas², ¹*Department of Ceramic and Materials Engineering*, ²*Johnson & Johnson Corporate Biomaterials Center*.

Ultrafine hydroxyapatite [HAp, Ca₁₀(PO₄)₆(OH)₂] powders were synthesized by the mechanochemical-hydrothermal method in a unique emulsion system consisting of salt solution as the water phase, petroleum ether (PE) as the oil phase and biodegradable Tomadol 23-6.5 as the nonionic surfactant. (NH₄)₂HPO₄ and Ca(NO₃)₂ or Ca(OH)₂ were used as the phosphorus and calcium sources, respectively. The effects of the emulsion composition on the stoichiometry, crystallinity and thermal stability of final products were studied.

11:45 Oxygen Plasma Treatment of Poly(dimethylsiloxane) Stamps, B. Langowski and K. Uhrich, *Dept. of Chemistry*.

Poly(dimethylsiloxane) (PDMS) substrates are oxygen plasma-treated to ensure microcontact printing, or stamping, of aqueous protein solutions onto biocompatible polymers, such as poly(methyl methacrylate). The influence of plasma-treatment on the PDMS stamps was evaluated using X-ray photoelectron spectroscopy and scanning electron microscopy.

12:00 Dynamics of Electron-induced Decomposition of CF₂Cl₂ and CCl₄ Co-Adsorbed with Water (Ice), N. S. Faradzhev¹, C. C. Perry², D. O. Kusmierek¹, D. H. Fairbrother², and T. E. Madey¹, ¹*Department of Physics and Astronomy*, ²*Johns Hopkins University*.

We compare the dynamics of decomposition and subsequent chemistry induced by ionizing radiation (electrons or x-rays) for two environmentally-important halocarbon molecules: CF₂Cl₂ and CCl₄. The molecules are adsorbed alone and co-adsorbed with water ice on a metal surface at low temperatures (25K and 100K). Temperature Programmed Desorption (TPD), Reflection Absorption Infrared Spectroscopy (RAIRS) and X-ray Photoelectron Spectroscopy (XPS) have been utilized. TPD data reveal the rapid decomposition of both halocarbon molecules under electron bombardment. The rate of their dissociation increases in the water environment. The highest cross-sections of halocarbon decomposition are $1.0 \pm 0.1 \times 10^{-15} \text{ cm}^2$ for CF₂Cl₂ and $2.5 \pm 0.1 \times 10^{-15} \text{ cm}^2$ for CCl₄. RAIRS and XPS studies allow us to identify reaction products of decomposition in the film. Generation of Cl⁻ and F⁻ anions in halocarbon/water film and production of H₃O⁺, CO₂ and COX₂ (X: F for CF₂Cl₂, and Cl for CCl₄) and C₂Cl₄ (for CCl₄), are observed using either electrons or Al K α x-ray photons as the primary source of ionizing radiation. The results provide evidence for the important role of a polar medium (water ice) in halocarbon decomposition, which proceeds via dissociative attachment (DA) of low energy secondary electrons pre-solvated by the water matrix.

1:45 Highlight presentation - Exploring the Limits of Transistor Scaling with Electron Microscopy, David Muller, *Bell Labs, Lucent Technologies*.

The smallest features on transistors used in computer circuits today have approached atomic dimensions: the SiO₂ gate oxides are between 5 and 8 silicon atoms thick and the concentration of dopant atoms has increased to the point that electrically inactive dopant clusters as small as a few atoms have become common enough to affect device performance. We have used atomic-resolution scanning transmission electron microscope with single atom sensitivity to identify the size, structure and distribution of clusters responsible for the saturation of charge carriers [1] and address the question of how many atoms are needed before the SiO₂ gate oxide loses its bulk properties. This puts a fundamental limit of 0.7 nm on the oxide thickness in order for the bulk SiO₂ properties to be achieved [2], and provides a challenge for the design of replacement gate dielectrics, many of which contain a few monolayers of SiO₂.

[1] P. M. Voyles, D. A. Muller, J. L. Grazul, P. H. Citrin, and H.-J. Gossmann, *Nature*, 416 p. 826 (2002).

[2] D. A. Muller, T. Sorsch, S. Moccio, F. H. Baumann and G. Timp, *Nature*, 399, p. 758 (1999).

2:15 Nucleation, Growth, and Structure of Alternative Gate Oxides, M. M. Frank^{1,4}, S. Dörmann², M.-T. Ho², Y. J. Chabal^{1,2,3}, S. Sayan¹, E. Garfunkel¹, G. D. Wilk⁴, and M. L. Green^{4,5}, ¹*Dept. of Chemistry*, ²*Dept. of Physics and Astronomy*, ³*Dept. of Biomedical Engineering*, ⁴*Agere Systems*, ⁵*IMEC, Belgium*.

The growth mechanisms, structure, and thermal behavior of atomic layer deposited (ALD) and chemical vapor deposited (CVD) Al₂O₃ and HfO₂ high-k dielectrics on silicon are studied by *in situ* and *ex situ* infrared spectroscopy. We follow chemisorbed species (e.g. -OH, -H, organic groups) and dielectrics with submonolayer sensitivity and detect defects and contaminants in the films formed. Based on these results, we have developed a novel method to activate hydrogen-terminated silicon for oxide deposition, namely using extended metal precursor pre-exposure, and to minimize the formation of interfacial SiO₂, namely by initiating growth at room temperature.

2:30 Band Alignment Issues of High-K Gate Stack Structures, S. Sayan¹, R.A. Bartynski², M. Croft², T. Emge¹ and E. Garfunkel¹, ¹*Dept. of Chemistry*, ²*Dept. of Physics and Astronomy*.

In this work we describe recent results using photoemission, inverse photoemission, xray absorption (XAS) and electrical methods to examine the densities of states above and below the Fermi energy of ultrathin HfO₂ and ZrO₂ films. The composition, structure and phase of the as-deposited and annealed films have also been studied by XRD, XAS, and ion scattering.

2:45 Nanochemistry of H, O₂ and H₂O at 3C-SiC Surfaces, F. Amy¹, Y. Chabal², ¹*Princeton University*, ²*Dept. of Chemistry and Dept. of Biomedical Engineering*.

While H is well known to passivate Si surfaces and SiO₂/Si interfaces, it induces a metallic state on the clean or water oxidized 3C-SiC surfaces. Hydrogenated 3C-SiC surface exposed to O₂ clearly shows that oxygen atoms are inserted below the top surface without any loss in the H coverage.

3:30 Tailoring of SAW Properties of ZnO-based Multilayer Structures, Y. Chen, K. Wu, N. W. Emanetoglu, Y. Lu, *Dept. of Electrical and Computer Engineering*.

ZnO thin films with high piezoelectric coupling coefficients are widely used for high frequency and low loss surface acoustic wave (SAW) devices. The SAW properties, including velocity dispersion and piezoelectric coupling, of $Mg_xZn_{1-x}O$ ($0 < x < 0.35$) films and ZnO/ $Mg_xZn_{1-x}O$ multilayer structures on r-plane sapphire are investigated using the transfer matrix method. The SAW properties can be tailored by adjusting the Mg composition, as well as the ZnO to $Mg_xZn_{1-x}O$ thickness ratio of the multilayer structures.

3:45 Revisiting Ni Growth on W(111): Faceting, Thermal Stability, and Reactivity, Q. Wu^{1,2}, J. Kolodziej³, H. Wang^{1,2}, and T. E. Madey¹, ¹*Dept. of Physics and Astronomy*, ²*Dept. of Chemistry*, ³*Instytut Fizyk, Jagellonian University, Poland*.

Nanoscale features formed by nucleation of ultrathin Ni films on W(111) are studied using ultrahigh vacuum-STM, SXPS, LEED, and AES. Whereas a single monolayer (ML) of Ni covers W(111) uniformly, we find that multilayers of Ni (~5 ML) follow the Stranski-Krastanov growth mode, and form clusters and islands on Ni-covered W(111). Upon heating to ~600K, Ni clusters are found to aggregate into nanoscale pyramidal facets, which coexist with planar regions of Ni-covered W(111). This type of faceting is different from the metal-monolayer-induced faceting of W(111) seen for Pt, Pd, Ir and Rh monolayers: a single ML of Ni does not cause faceting of W(111). Thermal stability of Ni films on W(211) and W(111) are studied by SXPS, which indicates that alloy formation between Ni and W occurs above ~700K. The growth of multilayer Ni on clean W(111) is in contrast with the growth on S(4x4)/W(111) and a surfactant effect is suggested. Reactivity of Ni nanofacets and nanoclusters with oxygen and thiophene is also investigated.

4:00 Electronic Polarization at Surfaces and in Thin Films of Organic Molecular Crystals (OMC), E. Tsiper¹, Z. G. Soos², ¹*Dept. of Chemistry*, ²*Princeton University*.

Clouds of electronic polarization around charge carriers and associated polarization energies in OMC are affected by proximity to surfaces and interfaces. We evaluate polarization by treating individual molecules rigorously in a self-consistent field of other molecules. Atom-atom polarizability tensor is introduced to describe intra-molecular charge redistribution. We find quantitative agreements in charge carrier energetics with photoelectron and STM data. Calculations reveal significant differences in electronic polarization at surfaces, metal-organic interfaces, in thin organic layers, and in the bulk, leading to about +/- 0.5 eV transport gap variations across organic films.

4:15 Growth and Thermal Evolution of Surface Structure in Ternary Sn-Si-Cu(001) Films, L. V. Goncharova^{1,2}, A. V. Ermakov¹, D. V. Potapenko¹, B. J. Hinch¹, X. Zhang³, D. R. Strongin³, ¹*Dept. of Chemistry*, ²*Dept. of Physics and Astronomy*, ³*Temple University*.

The commercial "Direct Synthesis" of dimethyldichlorosilane is very prominent in the manufacture of silicone materials. The synthesis uses Cu as a catalyst, enabling a high yield of dimethyldichlorosilane and lower yields of other methylchlorosilanes. Other metals, including Sn, Zn and Al, are also used in low levels as reaction promoters to further enhance the product selectivity. In fundamental investigations of Sn on the Cu(001) and the Cu₂Si/Cu(001) surfaces, high-resolution helium atom scattering (HAS), low energy electron diffraction (LEED) and Auger electron spectroscopy (AES) have been

used to study the growth of submonolayer thick Sn films, and the thermal stability of these films. In addition, temperature programmed desorption (TPD) studies have indicated that Sn, coadsorbed with silicon and methyl, on Cu(001) was found to enable a new low temperature pathway for desorption of tetramethylsilane. The latter product does not require cracking of methyl groups (which is prominent on Sn-free surfaces); the absence of cracking is highly desirable for the “Direct synthesis.” Our structural analyses have implied that tetramethylsilane evolution does not occur on a single Sn-Si-Cu ternary surface. We propose that the active mechanism for $\text{Si}(\text{CH}_3)_4$ desorption occurs instead at the boundaries between Sn-Si-Cu $c(2 \times 2)$ and Sn-Cu $p(\sqrt{2} \times 3\sqrt{2})R45^\circ$ phases.

Abstracts for Posters

1. Development of Ultrafast Near Field Optical Microscopy, S. Lou, F. Zimmermann, R. Bartynski, *Dept. of Physics and Astronomy*.

We are developing an apertureless near field optical microscope with femtosecond time resolution. The design incorporates a scattering-type (apertureless) near-field optical microscope based on a tuning fork atomic force microscope and a pump-probe approach using a Ti:sapphire femtosecond laser. The goal is to image (acquire "movies" of) ultrafast dynamical processes of various nanosystems with nanometer spatial resolution and femtosecond time resolution.

2. Adsorption and Decomposition of Acetylene on Clean and Oxygen-covered Ir(210), W. Chen¹, I. Ermanoski¹ and T. E. Madey¹, H. H. Hwu² and J. G. Chen², ¹*Dept. of Physics and Astronomy*, ²*University of Delaware*.

The adsorption and decomposition of acetylene (C_2H_2) on clean and oxygen-covered Ir(210) have been investigated with TPD, AES, LEED and HREELS. C_2H_2 adsorbs dissociatively on Ir(210). The dominant surface hydrocarbon species formed upon adsorption of C_2H_2 at high coverage are mainly acetylide (CCH) and ethylidyne (CCH_3) while acetylide (CCH) dominates at low coverage. Upon annealing, both CCH and CCH_3 decompose to produce H_2 , and CCH_3 also decomposes to produce other intermediate species that undergo further decomposition at higher temperatures to produce H_2 and leave C on the surface. Oxygen pre-covered Ir(210) affects the C_2H_2 decomposition pathways. We make use of AES line shapes to provide new information about the surface chemistry of acetylene on Ir(210). The HREELS data give complementary information to TPD and AES results.

3. Structural, Electronic and Catalytic Properties of Clean and Overlayer-Covered Ir(210), I. Ermanoski¹, W. Chen¹, M. J. Gladys¹, J. S. Quinton¹, T. E. Madey¹, M. Ulrich², and J. E. Rowe², ¹*Dept. of Physics and Astronomy*, ²*North Carolina State University*.

We report results on the structure, morphology, electronic and catalytic properties of the Ir(210) surface – clean as well as covered with gaseous and metallic overlayers. The atomically rough Ir(210) surface is morphologically unstable: When Ir(210) is covered with more than 0.6 ML of oxygen and annealed, pyramidal facets exposing {110} and {311} surfaces develop on the initially planar surface. We have used a variety of methods to characterize this surface, including LEED, STM and high resolution soft X-ray photoelectron spectroscopy (HRSXPS) using synchrotron radiation. To prepare an oxygen-free faceted surface, we use catalytic CO oxidation at ~500 K to react the oxygen off and “freeze” the surface in its pre-prepared faceted state. HRSXPS has been employed to investigate core-level features of all the surfaces mentioned. All of the surface components (first, second and third layer peaks) are identified with core-level shifts positioned at higher binding energies with respect to the bulk. Using TPD we find evidence for structural sensitivity in a surface reaction, i.e. differences in the chemical reactivity of on the planar and faceted surfaces. Overlayers of Pd and Pt exhibit structural changes upon

annealing, and HRXPS measurements show changes in the core-level properties of the overlayers.

*Supported by US DOE and ARO.

4. Electron- and Photon-stimulated Desorption of Alkali and Alkaline-earth Atoms from a Lunar Basalt Surface and a Model Mineral Surface, B. V. Yakshinskiy and T. E. Madey, *Dept. of Physics and Astronomy*.

Recent results on an investigation of source mechanisms for the origin of alkali atoms in tenuous planetary atmospheres (e.g., the Moon and the planet Mercury) are reported. The experiments have included electron- and photon-stimulated desorption and ion sputtering of alkali atoms from a model mineral surface (SiO_2) and from a lunar basalt sample. Whereas the concentrations of alkaline earth atoms (Ca, Mg) are much higher than those of Na, K in lunar soils, the atmosphere is dominated by Na, K. A comparison is made between desorption efficiency of monovalent alkalis (Na, K) and divalent alkaline earths (Ba, Ca).

5. TPD and STM Studies of Chlorosilane Desorption Mechanisms from Cl-exposed Cu/Si(111) Surfaces, D. V. Potapenko, S. E. Sysoev, A. V. Ermakov, D. Maithil, and B. J. Hinch, *Dept. of Chemistry*.

Complex desorption kinetics of SiCl_2 from Cl-covered Cu/Si(111) surfaces were investigated by TPD experiments. The results indicated an active role of chlorine-free sites in the SiCl_2 desorption process. We also report on STM studies of the Cl-covered Cu/Si(111) surfaces, following low temperature ($\sim 450^\circ\text{C}$) restructuring. We propose a desorption mechanism to explain the kinetics of the high-temperature desorption that draws on our knowledge of the atomic-level structures.

6. Nanometer Scale Thin Film Structure Analysis Using MeV He Ion Beams, L. S. Wielunski, *Dept. of Physics and Astronomy*.

Rutherford backscattering spectroscopy (RBS) using MeV He ions from the Rutgers ion accelerator (1.7MV Tandetron) is applied to study the composition and structure of thin film materials on a nanometer scale. The RBS spectrum provides information about thickness and atomic composition of thin films. Typical depth of analysis is up to 500-800nm and the standard depth resolution is about 20nm. The depth resolution can be improved in a number of ways, if necessary. The RBS technique can be combined with the ion channeling effect in order to study crystal quality of single crystal materials (including epitaxial structures) and impurity atom location in doped or contaminated structures.

7. Thermal Properties of Cerium Oxides as Potential High-k Dielectrics, R. Barnes¹, T. Nishimura², T. Gustafsson¹, E. Garfunkel³, ¹*Dept. of Physics and Astronomy*, ²*AIST, Tsukuba, Japan*, ³*Dept. of Chemistry*.

We study the characteristics of cerium oxides over SiO_x -terminated Si(100) to search for a possible new MOSFET gate dielectric. SiO_2 is the traditional gate dielectric, but problems arise when a transistor is scaled below a minimum size. Cerium oxides are promising for this application as they are expected to be stable over silicon substrates, and have a high dielectric constant. We grow the films by Physical Vapor Deposition; we

present data regarding the films' thermal stability using X-Ray Photoelectron Spectroscopy, Atomic Force Microscopy, and Medium Energy Ion Scattering.

8. Structural Characteristics of $Mg_xZn_{1-x}O$ Films Grown on R-plane Sapphire Substrates, G. Saraf, S. Muthukumar, J. Zhong, Y. Chen, Y. Lu, *Dept. of Electrical and Computer Engineering.*

ZnO and its ternary compound $Mg_xZn_{1-x}O$ films are promising to photonics and electronics. ZnO has a direct energy bandgap of 3.32eV which increases to 4.0eV at room temperature, with increase in Mg composition (upto~33%) in $Mg_xZn_{1-x}O$. Thus it can be used in ZnO based heterostructures. $Mg_xZn_{1-x}O$ grows with a wurzite structure on R-Sapphire, when a thin buffer of ZnO is used. Mg incorporation causes expansion in the unit cell leading to stress/strain in the as-grown film. This is evident from the peak broadening in the $\Delta 2\theta$, and the tilt from the broadening in $\Delta\omega$.

9. Wet Chemical Etching of ZnO Films Grown on R-Sapphire, J. Zhu, N. W. Emanetoglu, Y. Chen, Y. Lu, *Dept. of Electrical and Computer Engineering.*

The wet chemical etching process has been developed to etch the epitaxial ZnO films grown on R-sapphire. Different etching solutions have been used to generate steep etching profile and better surface morphology. Instead of photoresist, Al is used as the etching mask, which improves the etching profiles.

10. SAW Characteristics in Piezoelectric Materials Modified by ZnO Nanotips, Z. Zhang, W. Pan, S. Muthukumar, Y. Chen, Y. Lu, *Dept. of Electrical and Computer Engineering.*

In contrast with the newly reported wide bandgap GaN and SiC nanowires, which have random distribution in orientation and size, the ZnO nanotips arrays are oriented in a single direction, uniform in size and have a regular array distribution. The ZnO nanotips are grown on piezoelectric substrates using MOCVD. Its effects on SAW Characteristics have been analyzed.

11. Bulk Acoustic Wave Characteristics in Piezoelectric $Mg_xZn_{1-x}O$ Films, R. H. Wittstruck¹, X. Tong¹, N. W. Emanetoglu¹, J. Zhu¹, Y. Lu¹, A. Ballato², ¹*Dept. of Electrical and Computer Engineering,* ²*U. S. Army Communications-Electronics Command, Fort Monmouth.*

Piezoelectric thin film ZnO and its ternary alloy $Mg_xZn_{1-x}O$ have broad applications in transducers, resonators and filters. In this work, we present a new bulk acoustic wave (BAW) structure consisting of Al/ $Mg_xZn_{1-x}O$ /n+ - ZnO/r-sapphire, where Al and n+ type ZnO serve as the top and bottom electrode, respectively. The BAW characteristics are tailored when the Mg composition changes in the piezoelectric $Mg_xZn_{1-x}O$ films.

12. Channel Mobility Study of 4H-SiC Lateral JFET, P. Sannuti, X. Li, F. Yan, K. Sheng, J. H. Zhao, *Dept. of Electrical and Computer Engineering.*

Interface defects have limited 4H-SiC MOS-based FET channel mobility to less than 40-50 $cm^2/V.s$ after more than 10 years improvement. Junction-based FET, therefore, presents an excellent opportunity. This paper will report the realization of a record high channel mobility of 398 $cm^2/V.s$ for 4H-SiC lateral junction FET. The fabrication and

characterization as well as computer modeling results will be presented. The application of this very high channel mobility will also be discussed.

13. Understanding Response in TDDFT, F. Zhang, N. T. Maitra, K. Burke and R. J. Cave, *Dept. of Chemistry*.

Use of time-dependent density functional theory to calculate excitations has become standard in quantum chemistry and solid-state physics. In practice, when one uses an adiabatic approximation (such as ALDA), all the double (and multiple) excitations are missing. In our work, we show what kind of frequency-dependent behavior the exchange-correlation kernel must have in order to capture the missing double excitations.

14. A Model Description of Surface Second Harmonic Generation at Hydrogen Covered Si(001) Surface, M. B. Yilmaz, A. Rajagopal, F. Zimmermann, *Dept. of Physics and Astronomy*

Surface Second Harmonic Generation (SSHG) is an extremely valuable tool for studying the symmetries and geometrical and electronic structures of surfaces. In particular, it can be used as a sensitive, time resolved, non-invasive, in-situ probe for determining hydrogen coverage on silicon surfaces. We present a detailed experimental study of SHG from hydrogen covered Si(001) surface and a statistical mechanical model that can explain the observed dependence of SHG efficiency on hydrogen coverage.

15. The Local Density Approximation Can Yield Accurate Excitations to Rydberg States, A. Wasserman, N.T. Maitra, and K. Burke, *Dept. of Chemistry*.

We show how, in spite of its incorrect asymptotic behavior, the local density approximation to the Kohn-Sham potential can yield accurate optical spectra. The oscillator strengths associated with exact Rydberg excitations appear in the LDA spectrum as continuum contributions with about the right optical intensity. We illustrate this for the case of atomic Neon.

16. Nano-crack Growth by Ar⁺ Implantation with H⁺ Plasma Processing for SOI Exfoliation, B. Chen, A.Y. Usenko, W. N Carr, *NJIT*.

Ar⁺ ions were implanted into Si(100) at energy ranging from 30 KeV to 200 KeV and dose from 1×10^{15} to 1×10^{16} cm⁻². To avoid amorphization, the samples were thermally insulated and the beam current was maintained high enough (about 3mA/cm²). After implantation, pieces of these samples were subjected to thermal annealing at temperature ranging from 200°C to 800°C. The evolution of microstructure of these samples was investigated by TEM. In the annealed samples, Argon clusters are found in either 2-D cavities (Nano-cracks) or 3D cavities (bubbles). Then, these samples were processed by H⁺ plasma. Nano-cracks and bubbles will help trapping H diffused from the surface. We show that 2D cavities are more effective nucleation sites for hydrogen platelets than 3D cavities. After H⁺ plasma processing, these samples were annealed again. We can find that cracks grow along the direction parallel to the surface.

17. Unoccupied Electronic States of Ag/Al(100), J. F. Veyan^{1,2}, P. Häberle², W. Ibañez², R. Bartynski³, ¹*Departamento de Física, Universidad Católica, Valparaiso, Chile*,

²*Departamento de Física, Universidad Técnica, Valparaiso, Chile,* ³*Department of Physics and Astronomy.*

Using inverse photoemission spectroscopy (IPS) we have studied the empty electronic states of ultrathin Ag overlayers on the Al(100) surface. We find evidence for metallic quantum well (MQW) electronic states that are confined to the Ag film and change energy as a function of Ag film thickness. The origin of these states and a simple model that describes their behavior will be presented.

18. Comparative Study of Bioactive Bone Cement surfaces by SEM and NSOM, R. Vargas-Coronado¹, J. V. Cauich-Rodríguez¹, L. F. Garfias² ¹*Centro de Investigación Científica de Yucatán A.C, Mérida, Yucatán, México,* ²*Lucent Technologies.*

Cell interaction with biomaterials is greatly enhanced by the presence of charged substrates, topography and the presence of bioactive compounds. In this work, bone cements, prepared with functionalized methacrylates and hydroxiapatite, were studied by various surface characterization techniques. SEM and EDX analysis revealed poor distribution of the ceramic while an NSOM study enables us to study surface topography and interactions of the surface with simulated body fluid for several hours.