March 2002 DCP Program and Special Focus Topics

Table of Contents: pg i of ii (sessions in the Indiana Convention Cntr)

Nonlinear Spectroscopy and Molecular Choreography
Organized by David M. Jonas Location: Room 212
Session A32. Mon. 08:00, titles/times on pg. 1, abstracts in Bulletin
Session B32. Mon. 11:00, titles/times on pg. 2, abstracts in Bulletin
Session D32. Mon. 14:30, titles/times on pg. 2, abstracts in Bulletin
Session F32. Tues. 08:00, titles/times on pg. 3, abstracts in Bulletin
Session G32. Tues. 11:00, titles/times on pg. 3-4, abstracts in Bulletin

General Session on Chemical Physics of Complex Systems Loc: Rm 211
Session A31. Monday 08:00, titles/times on pg. 4-5, abstracts in Bulletin

Progress in Heterogeneous Catalysis, Fuel Cells, and Chemical Sensors (w FIAP) *Org. by A. Bogicevic, J. J. Zinck, and D. W. Goodman,* Location: Sagamore 7
Session F8. Tues. 08:00, titles/times on pg. 6 , abstracts in Bulletin
Session L8. Wed. 08:00, titles/times on pg. 6-7, abstracts in Bulletin

Chemical and Physical Properties of Supported and Isolated Metal Nanoclusters *Organized by Scott L. Anderson* Location: Room 211
Session F31. Tues. 08:00, titles/times on pg. 7-8, abstracts in Bulletin
Session G31. Tues. 11:00, titles/times on pg. 8, abstracts in Bulletin.
Session J31. Tues. 14:30, titles/times on pg. 8-9, abstracts in Bulletin.
Session L31. Wed. 08:00, titles/times on pg. 9, abstracts in Bulletin.

Division of Chemical Physics Business Meeting Tuesday 17:30, Rm. 211

Protein Dynamics (w DBP)
Organized by Norbert Scherer and Joan Shea Location: Room 212
Session J32. Tues. 14:30, titles/times on pg. 10, abstracts in Bulletin
Session L32. Wed. 08:00, titles/times on pg. 10-11, abstracts in Bulletin
Session M32. Wed. 11:00, titles/times on pg. 11-12, abstracts in Bulletin
Session Q32. Wed.14:30, titles/times on pg.12 , abstracts in Bulletin
Session S32. Thurs. 08:00, titles/times on pg. 12, abstracts in Bulletin

Table of Contents: pg ii of ii (sessions in the Indiana Convention Cntr)

General Session on Surface Science Location: Rm 211

Session S31. Thurs. 08:00, titles/times on pg. 13, abstracts in Bulletin

Vibronic Chemistry in Isolated Molecules, at Surfaces and in Solution

Organized by Martin Gruebele and Alec Wodtke Location: Room 212

Session T32. Thurs.11:00, titles/times on pg. 13-14, abstracts in Bulletin

Session U32. Thurs. 14:30, titles/times on pg. 14, abstracts in Bulletin

Session W32. Fri. 08:00, titles/times on pg. 15, abstracts in Bulletin

Session X32. Fri. 11:00, titles/times on pg. 15, abstracts in Bulletin

The Physical and Electronic Structure of Conjugated Polymers: From Photophysics to Devices *Organized by Ben Schwartz* Location: Room 208

Session T28. Thurs.11:00, titles/times on pg. 16, abstracts in Bulletin

Session U28. Thurs.14:30, titles/times on pg. 17, abstracts in Bulletin

Session W28. Fri. 08:00, titles/times on pg. 17, abstracts in Bulletin

Session X28. Fri. 11:00, titles/times on pg. 18, abstracts in Bulletin

Physics of Chemically Modified Interfaces (w DMP)

Organized by Eric Borguet Location: Room 211

Session T31. Thurs. 11:00, titles/times on pg. 18-19, abstracts in Bulletin

Session U31. Thurs. 14:30, titles/times on pg. 19-20, abstracts in Bulletin

Session W31. Fri. 08:00, titles/times on pg. 20, abstracts in Bulletin

Session X31. Fri. 11:00, titles/times on pg. 21, abstracts in Bulletin

New Techniques, Applications and Instruments in X-Ray Absorption Spectroscopy (w GIMS) *Org. by T. Guo, R. Schoenlein, and J. Rehr* Loc: Room 106

Session W13. Friday 08:00, titles/times on pg. 21-22, abstracts in Bulletin

Session X13. Friday 11:00, titles/times on pg. 22-23, abstracts in Bulletin

Division of Chemical Physics Poster Session (in Poster Session III.)

Session H33. Tues.14:00, Exhibit Hall D, Indiana Convention Center

March 2002 DCP Special Focus Topics and General Sessions

Nonlinear Spectroscopy and Molecular Choreography (DCP)

The term molecular choreography is borrowed from spin choreography in NMR and emphasizes the control we exert over the molecular dance we see in a nonlinear spectroscopic experiment. These sessions about making and watching molecules dance covers both experimental and theoretical aspects of nonlinear molecular spectroscopy, coherent molecular control, and the molecular dances in the elementary steps of chemical reactions.

Organizer: David M. Jonas, Department of Chemistry and Biochemistry, University of Colorado at Boulder

Session A32. Two Dimensional Nonlinear Spectroscopy.
Monday morning, 08:00, 212, Indiana Convention Center

08:00 A32.001 Two-Dimensional Vibrational Spectroscopy of Molecular Dynamics in Solution
Andrei Tokmakoff (MIT, Department of Chemistry)

08:36 A32.002 Simulations of the IR Photon Echo Response in Water
Andrei Piryatinski, Chris Lawrence, James L. Skinner (Department of Chemistry, University of Wisconsin-Madison)

08:48 A32.003 The lineshape function for the vibrational four-wave mixing spectroscopy:beyond stochastic modeling
Jaeyoung Sung, Robert J. Silbey (Department of Chemistry, Massachusetts Institute of Technology)

09:00 A32.004 Correlated Transition Energy Fluctuations Studied by Two-Dimensional Vibrational Spectroscopy of Coupled Vibrations
Nurettin Demirdöven, Munira Khalil, Andrei Tokmakoff (Department of Chemistry, Massachusetts Institute of Technology, Cambridge MA 02139)

09:12 A32.005 Dispersive and Dipolar Solvent-Solute Interactions of Acetone and Acetonitrile
George Devendorf (Indiana Academy, Ball State University)

09:24 A32.006 Chemical Measurement by Coherent Multi-dimensional Vibrational Spectroscopy
John Wright (University of Wisconsin- Madison)

10:00 A32.007 Direct observation of intramolecular vibrational energy flow down a hydrocarbon chain using 3D IR-Raman spectroscopy.
Andrei Pakoulev, Zhaohui Wang, Dana Dlott (University of Illinois at Urbana-Champaign)

10:12 A32.008 Directly probing the solvent response with third-order nonresonant femtosecond spectroscopy following resonant initiation of solvation and proton transfer
David Underwood, Sarah Schmidtke, David Blank (University of Minnesota)

10:24 A32.009 Two-Color Three Pulse Photon Echo Peak Shift Spectroscopy
Bradley Prall, Ritesh Agarwal, Abbas Rizvi, Mino Yang, Graham Fleming (Department of Chemistry, University of California, Berkeley and Physical Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley, California)

10:36 A32.010 Disentangling polar and non-polar solvation with 2D spectra
Anchi Yu, John Hybl, Darcie Farrow, David Jonas (Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309-0215)

Session B32. Nonlinear Computing and Polarization Spectroscopy.
Monday morning, 11:00, 212, Indiana Convention Center

11:00 B32.001 Time-Frequency Resolved Four-Wave Mixing: From Control to Computing
V. A. Apkarian (Department of Chemistry, University of California, Irvine)

11:36 B32.002 Femtosecond laser control of multiphoton processes and nonlinear optical computation.
Katherine Walowicz, Igor Pastirk, Vadim Lozovoy, Matthew Comstock, Evgeny Sudachenko, Marcos Dantus (Michigan State University)

11:48 B32.003 Harnessing optical and chemical nonlinearity for nanofabrication
John Fourkas, Tommaso Baldacchini, Huzhen Chen, Richard Farrer (Department of Chemistry, Boston College), Michael Naughton, Joel Moser (Department of Physics, Boston College)

12:00 B32.004 A Coupled-Oscillator Model for Molecular Chirality in Nonlinear Optics
M. A. Belkin (Department of Physics, University of California, Berkeley), C. Flytzanis (Laboratoire d'Optique Quantique du CNRS, Ecole Polytechnique, France), Y. R. Shen (Department of Physics, University of California, Berkeley)

12:12 B32.005 Nonlinear Optical Chiral Responses from Surface Monolayers and Bulk
S. H. Han, M. A. Belkin, Na Ji, Y. R. Shen (Department of Physics, University of California, Berkeley)

12:24 B32.007 Polarization-Resolved Four-Wave Mixing Spectroscopy as a Probe of Intramolecular Dynamics
Patrick H. Vaccaro (Department of Chemistry, Yale University)

13:00 B32.008 Calculations of nonlinear Raman spectroscopy of Xe
Jianshu Cao (MIT)

13:12 B32.009 Absorption Anisotropy Studies of Ultrafast Dynamics in Transition Metal Chromophores
James McCusker (Department of Chemistry, Michigan State University)

13:24 B32.010 The Interaction Between Rotating Dipoles
Y.C. Lan, R. Tao (Temple U., Philadelphia, PA)

Session D32. Molecular Dynamics From Nonlinear Spectroscopy.
Monday afternoon, 14:30, 212, Indiana Convention Center

14:30 D32.001 Using Thz Spectroscopy to Probe Intramolecular Electron Transfer and Solvent Dynamics
Charles Schmuttenmaer (Yale University, Department of Chemistry)

15:06 D32.002 Terahertz Spectroscopy of Biomolecules
Timothy Korter, David Plusquellic, Angela Hight Walker, Edwin Heilweil (National Institute of Standards and Technology, Physics Laboratory, Gaithersburg, MD 20899)

15:18 D32.003 Low Frequency Raman Modes of Biotin
Mary N. Boyden, Timothy M. Korter, Maritoni Litorja, Angela R. Hight Walker (National Institute of Standards and Technology, Physics Laboratory, Gaithersburg, MD 20899)

15:30 D32.004 Aqueous Solvation at Biomimetic Interfaces
Alexander V Benderskii, Kenneth B Eisenthal (Department of Chemistry, Columbia University)

15:42 D32.005 Surface mediated solvation at liquid-hydrophilic solid interfaces studied by second harmonic generation
Xiaoyi Zhang (Chemical Physics Program, University of Maryland), Esenturk Okan, Robert Walker (Department of Chemistry, University of Maryland)

15:54 D32.006 Melting at Alkyl Side Chain Comb Polymer Interfaces
Keshav Gautam, Ali Dhinojwala (Department of Polymer Science, The University of Akron)

16:06 D32.007 Vibrational Sum-Frequency Spectroscopy of Vapor/H_2O:HOD:D_2O Interfaces
Elizabeth Raymond (Department of Physics and Materials Science Institute, University of Oregon), Teresa Tarbuck, Geraldine Richmond (Department of Chemistry and Materials Science Institute, University of Oregon)

16:18 D32.008 New Features in the Vibrational Coherence Dynamics of Liquids and Proteins
Hugh Hubble, Tianshu Lai, Jianwen Jiang, Mark Berg (Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC 29208)

16:30 D32.009 Two Dimensional Ultrafast Infrared Vibrational Echo Studies of Condensed Matter Dynamics and Interactions, Michael D. Fayer (Department of Chemistry, Stanford University, Stanford, CA 95305)

Session F32. Nonlinear Spectroscopy and Molecular Choreography.

Tuesday morning, 08:00, 212, Indiana Convention Center

08:00 F32.001 Using Coherent Control to Probe the Electronic Properties of Molecules
Robert J. Gordon (Department of Chemistry, University of Illinois at Chicago)

08:36 F32.002 Variational approach to the optimal control of time-averaged quantities in open quantum systems
Martin Garcia, Ilia Grigorenko (Institute for Theoretical Physics, Freie Universitaet Berlin)

08:48 F32.003 A new tool for vibrational nonlinear spectroscopy: High resolution indirect pulse shaping in the infrared by parametric transfer
Howe-Siang Tan, Elmar Schreiber, Warren Warren (Princeton University)

09:00 F32.004 Pulsed Infrared Vibrational Population Control in Liquid-Phase Metal Carbonyls
Valeria D. Kleiman (Chemistry Department, University of Florida, Gainsville, FL 32611-7200 USA), Joseph S. Melinger (Electronics Science and Technology Division, Code 6812, Naval Research Laboratory), Edwin J. Heilweil (Optical Technology Division, National Institute of Standards and Technology)

09:12 F32.005 Making and Measuring Vibrational Wave Packets In Small Molecules Through Impulsive Non-Resonant Stimulated Raman Scattering
Thomas Weinacht, Randy Bartels, Oliver Monti, Steve Leone, Margaret Murnane, Henry Kapteyn (JILA)

09:36 F32.006 Measuring D_2^+ vibrational wavepackets with sub-femtosecond precision
P.B. Corkum (National Research Council of Canada, Ottawa, Ontario Canada)

10:12 F32.007 Ultrafast hot-electron-mediated surface/adsorbate dynamics probed by EUV light
Chi-Fong Lei, Ra'anan Tobey, Sterling Backus, Margaret Murnane, Henry Kapteyn (JILA, University of Colorado, Boulder, CO 80309-0440), Michael Bauer (Fachbereich Physik, University Kaiserslautern, Erwin Schroedinger Str. 46, 67663 Kaiserslautern, Germany)

10:24 F32.008 Methyl Dynamics in N-Methylacetamide
S. Rols, K. W. Herwig (Oak Ridge National Laboratory), H. N. Bordallo (Argonne National Laboratory), M. Barthes (Universite Montpellier 2)

10:36 F32.009 Noise spectroscopy of randomly modulated atoms
Jennifer Green, David White, Marvin Kemple, Gautam Vemuri (Physics Dept., IUPUI)

Suppl. F32.010 Strong friction limit in quantum mechanics: The quantumSmoluchowski equation
Joachim Ankerhold (Fakultaet fuer Physik, University of Freiburg, Germany), Philip Pechukas (Department of Chemistry, Columbia University, New York), Hermann Grabert (Fakultät für Physik, University of Freiburg, Germany)

Session G32. Nonlinear Spectroscopy, Single Molecules and Molecular Control.

Tuesday morning, 11:00, 212, Indiana Convention Center

11:00 G32.001 Single-Molecule Dynamics Induced by Tunneling Electrons
Tamar Seideman (National Research Council of Canada)

11:36 G32.002 Time-Resolved, Single-Photon Spectrometers Using Superconducting Tunnel Junctions
C.M. Wilson, L. Frunzio, D.E. Prober (Yale University)

11:48 G32.003 Density functional calculations of the adsorption of C_6H_5Cl/ Si(111) 7x7, and comparison with STM manipulation experiments.
M. F. G. Hedouin, R.E. Palmer (Nanoscale Physics Research Laboratory, School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham, B15 2TT, U.K.), Mats Persson (Department of Applied Physics, Chalmers/Goteborg University, S-41296 Goteborg, Sweden.)

12:00 G32.004 Broadband, Near-Field Extinction Spectra of Single Gold Nanoparticles
Alexander Mikhailovsky, Victor Klimov (Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM 87545), Soft-Matter Nanotechnology and Advanced Spectroscopy Team

12:12 G32.005 Photostability of Immobilized Luminescent Single Si Nanoparticles Under Infrared Femtosecond Irradiation
N Barry, O Akcakir, G Belomoin, E Gratton, M Nayfeh (Univ of Illinois at Urbana-Champaign)

12:24 G32.006 Fluorescence of Cascade Blue inside Nano-Sized Shells of Silicate
Agnes Ostafin, Matthew Siegel, Qiang Wang (University of Notre Dame), Hiroshi Mizukami (Wayne State University)

12:36 G32.007 Experimental Investigation of Second-Harmonic Generation from Nanoparticles
Jie Shan, Igor Stiopkin, Jerry Dadap (Columbia University), Georg Reider (Technical University of Vienna, Austria), Tony F. Heinz (Columbia University, New York, NY)

12:48 G32.008 Phase and amplitude control of multiple-order wave packet preparation processes: Evolutionary optimization and quantum information
Stephen R. Leone (JILA, National Institute of Standards and Technology and University of Colorado)

13:24 G32.009 Wavepacket Interferometry for Energy Transfer
Jeffrey A. Cina (Oregon Center for Optics and Dept of Chemistry, University of Oregon, Eugene, OR 97403), Dmitri Kilin, Travis S. Humble (University of Oregon)

13:48 G32.010 Optical Studies of a Novel Mixed-Metal (Silver-Gold) Layered Solid
C. L. Larochelle (Dickinson College, Dept. of Physics), H. H. Patterson (University of Maine, Dept. of Chemistry)

General Session on Chemical Physics of Complex Systems (DCP)

Session A31. Chemical Physics of Complex Systems.
Monday morning, 08:00, 211, Indiana Convention Center

08:00 A31.001 Diffusion of Dioxygen and Aromatic Hydrocarbons in n-Alkanes
Bruce Kowert, Kurt Sobush, Chantel Fuqua, Courtney Mapes (Dept. of Chemistry, St. Louis University)

08:12 A31.002 Hydrogen Storage in Sodium Alanates II: Low Pressure Rehydriding of NaH+Al to Na_3AlH_6
Gary G. Tibbetts, Gregory P. Meisner, Frederick E. Pinkerton, Charles H. Olk, Michael P. Balogh (Materials and Processes Lab, General Motors Ramp;D Center)

08:24 A31.003 Hydrogen Storage in Sodium Alanates I: Thermal Decomposition of Milled and Doped $NaAlH_4$
Gregory P. Meisner, Gary G. Tibbetts, Frederick E. Pinkerton, Charles H. Olk, Michael P. Balogh (General Motors R amp; D Center, MC 480-106-224, Warren, MI, 48090-9055)

08:36 A31.004 Analytical approaches in time-dependent nucleation: recent updates
Vitaly Shneidman (Department of Physics, NJIT, Newark, NJ 07102)

08:48 A31.005 New Extended Phases of Carbon Dioxide at High Pressures
Choong-Shik Yoo, Valentin Iota, Hyunchae Cynn, Jaehyun Park (Lawrence Livermore National Laboratory, Livermore, CA 94551), Malcolm Nicol, Holger Kohlmann (University of Nevada, Las Vegas, NV 89154)

09:00 A31.006 Ab initio Investigation of He^+ Bubble Formation in Solid Hydrogen
R. H. Scheicher, T. P. Das (SUNY Albany, Albany NY), K. Ishida, T. Matsuzaki, S. N. Nakamura, N. Kawamura (RIKEN, Wako-shi, Japan), K. Nagamine (KEK-MSL, Tsukuba, Japan; RIKEN)

09:12 A31.007 Effects of Gas Diffusion on Nucleation of Gas-Supersaturated Liquids
G.J. Brereton, X. Liu, S. Garrett (Michigan State University), J.R. Spears (Wayne State University)

09:24 A31.008 Effect of Adsorption on the Contact Angle: Water-Glass System
Ali Keshavarz (PhD Student), Charles A. Ward (Professor, APS member)

09:36 A31.009 Small Hydrophobic Molecules in Water: First Principles Simulations
Jeffrey C. Grossman, Andrew Williamson, Eric Schwegler, Giulia Galli (Lawrence Livermore National Laboratory, 7000 East Ave. L-415, Livermore, CA 94550)

09:48 A31.010 First-Principles Study of Influence of Intermolecular Bonding on Nuclear Quadrupole Interaction in Solid Halogens
D. D. Paudyal, M. M. Aryal, S. Byahut (Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal), Junho Jeong, R. H. Scheicher, T. P. Das (Dept. of Physics, SUNY Albany, Albany NY)

10:00 A31.011 Electronic structure study of Ti-Ni amorphous and crystalline alloys by Auger electron appearance potential spectroscopy
S.H. McKinney, A.R. Chourasia (Department of Physics, Texas Aamp;M University-Commerce, Commerce, TX 75429), A. Ishida Collaboration

10:12 A31.012 Theory of Nuclear Quadrupole Interactions in the Chemical Ferromagnet p-Cl-Ph-CH-N=TEMPO
Tina M. Briere (Inst. MAt. Res., Tohoku Univ., Japan), Junho Jeong (SUNY Albany, Albany, NY), N. Sahoo (Albany Medical College, Albany, NY; SUNY Albany, Albany, NY), T. P. Das (SUNY Albany), S. Ohira (RIKEN, Wako-shi, Japan), K. Nishiyama (KEK-MSL, Tsukuba, Japan), K. Nagamine (RIKEN; KEK-MSL)

10:24 A31.013 A Simple Surface Nucleation Model of Small Particle Melting Applied to Water in Silica Pores
Karl Unruh (University of Delaware)

10:36 A31.014 Nucleation near the spinodal in Yukawa fluids
G. Wilemski, J. -S. Li (Univ. of Missouri-Rolla)

10:48 A31.015 Temperature dependence of nucleation in Yukawa fluids
J.-S. Li, G. Wilemski (University of Missouri-Rolla)

Suppl. A31.016 Finite Size Scaling in Quantum Mechanics, Sabre Kais (Chemistry Dept., Purdue University)

Progress in Heterogeneous Catalysis, Fuel Cells, and Chemical Sensors (FIAP/DCP)

While the areas of catalyst, fuel cell (both PEM and SOFC), and gas sensor development are perhaps not normally grouped together, they actually have several key issues in common. All three areas rely on complex catalytic reactions on one or two separate electrodes, atomic and molecular transport on surfaces and in the bulk, and are all faced with issues of thermal and chemical stability under harsh oxidizing/reducing environments and large temperature variations. This focus session will provide an overview of the current state of the art in these fields, and a forum for comparisons of different approaches to common problem formulations. Experimental and theoretical papers are solicited on a wide variety of phenomena, including (but not limited to) the following areas:

Structural (e.g., microstructure, mechanical properties, durability)
Chemical (e.g., surface chemistry, micro- and macrokinetics, triple-point boundaries)
Transport (e.g., bulk and surface diffusion, ionic transport, dopant interactions)
Electronic (e.g., band-gap engineering, optical properties, nanostructures)
Methodology (e.g. combinatorics, computation, nanotechnology)

Authors are encouraged to stress the relevance of their work to technological and industrial problems. Materials of interest include metals, semiconductors, and ceramics, either in bulk or at surfaces or interfaces. Contributions based on all experimental, theoretical, and computational methodologies are welcome.

Organizers: Alexander Bogicevic, Scientific Research Laboratories, Ford Motor Co., Jennifer J. Zinck, HRL Labs, D. Wayne Goodman, Dept. of Chemistry, Texas A&M Univ.

Session F8. Progress in Sensors and Catalysis.
Tuesday morning, 08:00, Sagamore 7, Indiana Convention Center

08:00 F8.001 Sensors and Micromachined Devices for the Automotive and New Markets: The Delphi Delco Electronics MEMS Story.
James Logsdon (Delphi Delco Electronics Systems)

08:36 F8.002 Fiber-Optic Hydrogen Sensors Based upon Chromogenic Materials
Roland Pitts (National Renewable Energy Laboratory)

09:12 F8.003 A Balanced Hydrogen Gas Sensor Based on Pd/AlN/Si(111) structure
E.~F. McCullen, Wenjun Mo, H.~E. Prakasam, G.~W. Auner, R. Naik, S. Ng, L. Rimai (Wayne State Univ.)

09:24 F8.004 A Novel Modeling Framework for Heterogeneous Catalyst Design
Santhoji Katare, Aditya Bhan, James Caruthers, Nicholas Delgass, Jochen Lauterbach, Venkat Venkatasubramanian (School of Chemical Engineering, Purdue University, West Lafayette, IN 47907)

09:36 F8.005 Why is a noble metal catalytically active? The behavior of the oxygen/silver system as studied by DFT-GGA including effects of the environment.
Weixue Li, Catherine Stampfl, Matthias Scheffler (Fritz-Haber-Institut der MPG, D-14195 Berlin-Dahlem, Germany)

09:48 F8.006 Reasons for DFT inaccuracy in CO/Pt(111) system
Yashar Yourdshahyan, Ilya Grinberg, Andrew M Rappe (Department of Chemistry and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, Pa 19104-6323)

10:00 F8.007 First-Principles Study of CO Adsorption on Zirconia-Supported Copper
Andrew M. Rappe (Dept. of Chemistry and Laboratory for Research on the Structure of Matter, Univ. of Pennsylvania, Philadelphia, PA), Eric J. Walter (Dept. of Physics and Center for Piezoelectrics by Design, College of William and Mary, Williamsburg, VA), Steven P. Lewis (Dept. of Physics and Astronomy and Center for Simulational Physics, Univ. of Georgia, Athens, GA)

10:12 F8.008 Cooperative Enhancements in NO_x Chemisorption on Oxide Surfaces
K. C. Hass, W. F. Schneider (Ford Research Laboratory), M. Miletic, J. L. Gland (U. of Michigan)

10:24 F8.009 Characterization of Cu Mordenite deNOx Catalysts at Variable Si/Al Ratios, by NMR, TPD and Optical Spectroscopy, Robert F. Marzke (Department of Physics and Astronomy, Arizona State University, Tempe, AZ 85287-1504), Vitalii P. Petranovskii, Nina E. Bogdanchikova (Centro de Ciencias de la Materia Condensada, UNAM, Apdo. Postal 2681, 2280, Ensenada, B.C. Mexico)

10:36 F8.010 Reduction studies of CuO particles using in situ time-resolved x-ray diffraction
J. Y. Kim, J. C. Hanson, J. A. Rodriguez (Chemistry Dept., BNL, Upton, NY 11973)

Suppl. F8.011 Non-adiabatic Molecular Dynamics Simulation of the Ultrafast Electron Transfer from a Molecular Electron Donor to the TiO_2 Acceptor
Oleg Prezhdo, William Stier (Department of Chemistry, Univ. of Washington, Seattle WA 98195-1700)

Session L8. Progress in Sensors and Fuel Cells.
Wednesday morning, 08:00, Sagamore 7, Indiana Convention Center

08:00 L8.001 Fundamental principles of metal oxide based chemical sensors
Nicolae Barsan (Inst. of Phys. Theor. Chemistry, University of Tuebingen)

08:36 L8.002 Direct Observation of Metal-Oxide Interactions in Nanoscale Systems
Robert F. Klie, Kai Sun, Nigel D. Browning (University of Illinois at Chicago, 845 West Taylor Street, Chicago, IL 60607), Mark M. Disko (ExxonMobil Research and Eng. Co., Annandale, NJ 08801), J. Liu (Monsanto Company, St. Louis, Missouri 63167)

08:48 L8.003 First Principles Studies of Ultra-thin Pt Films on Chiral $SrTiO_3$ Surfaces
Aravind Asthagiri, David Sholl (Dept. of Chemical Engineering, Carnegie Mellon University)

09:00 L8.004 Nature and Strength of Defect Interactions in Cubic Stabilized Zirconia
Alexander Bogicevic (Ford Motor Company), Christopher Wolverton (Ford Research Laboratory)

09:12 L8.005 Enthalpies of Formation of Yttria- and Zirconia-Doped Ceria
Theresa Lee, Alexandra Navrotsky (University of California at Davis)

09:24 L8.006 Effect of Anion Sublattice Structure on Conductivity in Cubic Bismuth Oxides
Eric Wachsman (University of Florida)

09:36 L8.007 Neutron quasielastic scattering study of hydrogen diffusion in $ZrBe_2H_{1.5}$
Z. Chowdhuri (NIST Center for Neutron Research, Gaithersburg, MD 20899, and University of Maryland, College Park, MD 20742), R. L. Cappelletti, T. J. Udovic (NIST Center for Neutron Research)

09:48 L8.008 Improved Electrodes and Electrolytes for Polymer Electrolyte Fuel Cells
Tom Zawodzinski (Los Alamos National Lab)

10:24 L8.009 Quantum treatment of H adsorbed on a Pt(111) surface
Gustav Källen, Göran Wahnström (Department of Applied Physics, Chalmers University of Technology and Göteborg University, SE-412 96 Göteborg, Sweden)

10:36 L8.010 First Principles Investigation of Hydrogen Transport through Copper-Palladium Alloy Membranes.
Preeti Kamakoti (Dept. of Chemical Engineering, Carnegie Mellon University), David Sholl (Carnegie Mellon University and National Energy Technology Laboratory)

Chemical and Physical Properties of Supported and Isolated Metal Nanoclusters (DCP)

Supported metal nanoclusters are important in many catalysts and in other materials applications. It is known that the chemical and materials properties of supported clusters depend strongly on parameters such as cluster size, morphology, and oxidation state, and also on support properties such as defect structure and redox behavior, however, the origin of the effects is not understood. Recently, there have been major advances in the study of supported clusters using both deposition of size-selected clusters and controlled nucleation of clusters on supports. Simultaneously, new spectroscopic, diffraction, and imaging methods have been developed that allow detailed study of isolated clusters. This focus session will provide a forum for discussion and comparison of different approaches to probing the relationships between the physical, chemical, and materials properties of metal nanoclusters. Experimental and theoretical papers are solicited in any related area, including, but not limited to:

Deposition of energy and/or mass-selected clusters
Growth, mobility, properties of cluster on surfaces
Physical and chemical properties of isolated metal clusters
Nano-cluster-based catalysts or materials
Theory on clusters or cluster-support interactions

Organizer: Scott L. Anderson, Department of Chemistry, University of Utah

Session F31. Metal Nanoclusters: Physical Properties and Preparation.

Tuesday morning, 08:00, 211, Indiana Convention Center

08:00 F31.001 X-Ray Dichroism and Magnetometry Study of Supported Fe and Co Nanoparticles
C. Binns (Department of Physics amp; Astronomy, University of Leicester, Leicester LE1 7RH, UK)

08:36 F31.002 The Prospects for Cluster-Based Materials
Kit Bowen (Johns Hopkins University)

08:48 F31.003 Theoretical and Experimental Studies of the Structures of 12-, 13-, and 14-atom Bimetallic Ni/Al Clusters.
Eric F. Rexer, Eric K. Parks, Stephen J. Riley, Evgueni B. Krissinel (), Julius Jellinek (Argonne National Laboratory)

09:00 F31.004 Softlanding and stability of mass selected Ag clusters on Pt(111)
Wolfgang Harbich (Dep. Physique, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland)

09:36 F31.005 Production of Ultracold Sodium Clusters by Helium Nanodroplet Aggregation
Sascha Vongehr (University of Southern California, Los Angeles), Adi Scheidemann (Intelligent Ion, Seattle), Curt Wittig, Vitaly Kresin (USC)

09:48 F31.006 Dynamical simulation of cluster on the surface
W. Fan, D. Y. Sun (Institute of Solid State Physics, Academia Sinica, 230031-Hefei, P. R. China), X. G. Gong (Department of Physics, Fudan University, Shanghai 200433, P. R. China, and Institute of Solid State Physics, Academia Sinica, 230031-Hefei, P. R. China)

10:00 F31.007 Clusters at Surfaces: Deposition, Anomalous Diffusion. and Nanocatalysis
Uzi Landman (School of Physics, Geirgia Instituite of Technology, Atlanta, GA)

10:36 F31.008 Ab Initio Monte Carlo Simulations for Nanoscopic Lithium Systems at Different Temperatures
Sanwu Wang, S. J. Mitchell, P. A. Rikvold (Florida State University.)

Session G31. Metal Nanoclusters: Chemistry I.
Tuesday morning, 11:00, 211, Indiana Convention Center

11:00 G31.001 Guiding Principles in Nanocatalysis
Ulrich Heiz (University of Ulm, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany)

11:36 G31.002 CO oxidation on a single Pd atom supported on magnesia
Hannu Häkkinen, Uzi Landman (Georgia Institute of Technology, Atlanta, GA), Stephane Abbet, Ulrich Heiz (University of Ulm, Germany)

11:48 G31.003 Reaction of carbon monoxide and oxygen with small free gold clusters at cryogenic temperatures
Thorsten M. Bernhardt, Liana D. Socaciu, Jan Hagen, Maryam Elijazyfer, Ludger Woeste (Institute of Experimental Physics, Free University of Berlin, Arnimallee 14, D-14195 Berlin, Germany), Ueli Heiz (Department of Surface Chemistry and Catalysis, University of Ulm, D-89069 Ulm, Germany)

12:00 G31.004 In Situ Characterization of Supported Nanoparticles
D. Wayne Goodman (Texas A&M University)

12:36 G31.005 Bond energies of molecular fragments to clusters
Peter B. Armentrout, Rohana Liyanage (Chemistry Department, University of Utah)

12:48 G31.006 CO and O_2 adsorption on iridium clusters
Mats Andersson, Tobias Järvdalen, Per Nyström, Arne Rosén (Department of Experimental Physics, Chalmers University of Technology and Goteborg University, SE-41296 Goteborg, Sweden)

13:00 G31.007 Effects of cluster size, impact energy, and support state on the properties of Ni clusters on oxide supports.
Scott L. Anderson (University of Utah)

13:36 G31.008 Size-Specific Reactions of Simple Molecules on Copper Cluster Ions
Masahiko Ichihashi (Toyota Technological Institute, Ichikawa, Japan), Charlotte A. Corbett (University of Illinois at Urbana-Champaign, Urbana, IL), Tetsu Hanmura (Genesis Research Institute, Ichikawa, Japan), James M. Lisy (University of Illinois at Urbana-Champaign, Urbana, IL), Tamotsu Kondow (Toyota Technological Institute, Ichikawa, Japan)

Session J31. Metal Nanoclusters: Chemistry II.
Tuesday afternoon, 14:30, 211, Indiana Convention Center

14:30 J31.001 Infrared spectroscopy and temperature desorption spectroscopy of size-selected supported organometallic clusters
Atsushi Nakajima (Department of Chemistry, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama, 223-8522 Japan)

15:06 J31.002 Molecular-Dynamics Simulation of Solvation Forces Between Colloidal Nanoparticles
Yong Qin, Kristen Fichthorn (The Pennsylvania State University)

15:18 J31.003 The surface termination of RuO_2(110) at high pressure: implications for the oxidation catalysis on Ru
K. Reuter, Q. Sun, M. Scheffler (Fritz-Haber Institut, Berlin, Germany)

15:30 J31.004 Interaction of small molecules with soft-landed transition-metal nanoclusters
Junichi Murakami (Institute for Structural and Engineering Materials, National Institute for Advanced Industrial Science and Technology (AIST))

16:06 J31.005 Electric dipole measurements of metal - fullerene clusters:: structure and dynamics
Ph. Dugourd, R. Antoine, M. Broyer, I. Compagnon, D. Rayane (Universite Lyon 1)

16:18 J31.006 Preparing nanoparticle assemblies with number density gradients
Rajendra Bhat (Department of Chemical Engineering, North Carolina State University, Raleigh, NC 27695), Daniel Fischer (Material Science and Engineering Laboratory, National Institute for Standards and Technology, Gaithersburg, MD 20899), Jan Genzer (Department of Chemical Engineering, North Carolina State University, Raleigh, NC 27695)

16:30 J31.007 Size-Dependent Catalytic Reactions of Metal Clusters
Tamotsu Kondow (Toyota Technological Institute)

17:06 J31.008 Computer Simulations of Ni-Al Alloy Nanoclusters
Yaroslav Chushak, Lawrence S. Bartell (Dept. of Chemistry, Univ. of Michigan, Ann Arbor, MI 48109)

Session L31. Metal Nanoclusters: Spectroscopy and Structure.
Wednesday morning, 08:00, 211, Indiana Convention Center

08:00 L31.001 Infrared Spectroscopy of Mass-Selected Transition Metal Complexes
Michael Duncan (University of Georgia)

08:36 L31.002 Electric Field Deflection Studies of Nickel and Niobium Clusters
Mark Knickelbein (Chemistry Division, Argonne National Laboratory)

08:48 L31.003 Photoionization of alkali nanoclusters in a beam: Energy and temperature dependence
Vitaly Kresin, Kin Wong, George Tikhonov, Vitaly Kasperovich (University of Southern California)

09:00 L31.004 Trapped Ion Electron Diffraction: Probing Structural Changes in Nanoclusters
Joel H Parks (Rowland Institute for Science; Cambridge, Massachusetts)

09:36 L31.005 Electron Binding Energies of Anionic Magnesium Clusters and the Size-Induced Insulator-to-Metal Transition
Julius Jellinek, Paulo Acioli (Chemistry Division, Argonne National Laboratory, Argonne, IL 60439)

09:48 L31.006 Infrared Spectroscopy of Gas Phase Metal Clusters
Deniz van Heijnsbergen, Gerard Meijer (FOM Institute Rijnhuizen, Edisonbaan 14, 3439 MN Nieuwegein, The Netherlands), Michael Duncan (Dept. of Chemistry, Univ. of Georgia, Athens, GA 30602), Gert von Helden (FOM Institute Rijnhuizen, Edisonbaan 14, 3439 MN Nieuwegein, The Netherlands)

10:00 L31.007 Structure, stability, dissociation, and vibration of Ni_n clusters
Valeri G. Grigoryan, Michael Springborg (Physical Chemistry, University of Saarland, 66123 Saarbrücken, Germany)

10:12 L31.008 LCAO Density-functional study of platinum clusters
Edoardo Apra (EMSL - Pacific Northwest National Laboratory), Alessandro Fortunelli (ICQEM - CNR)

Division of Chemical Physics Business Meeting.
Tuesday afternoon, 17:30, 211, Indiana Convention Center

All DCP members encouraged to attend.

Protein Dynamics (DCP/DBP)

A full understanding of protein function and molecular recognition requires a description of the system or complex that extends beyond the static three-dimensional picture provided by "traditional" structure determination approaches. This Symposium concentrates on experimental, theoretical and computational studies and approaches that are at the forefront of probing and analyzing the dynamic behavior of proteins and protein-ligand complexes. The individual sessions are organized around the following broad topics: Quantum dynamics and electron transfer processes; Long time dynamics; Time-resolved folding; Protein-Ligand dynamics including single molecule behavior; Ion Channel dynamics. Papers are solicited in all areas related to protein dynamics.

Organizers: Norbert Scherer, Dept. of Chemistry and Inst. for Biophysical Dynamics, The Univ. of Chicago and Joan-Emma Shea, Dept. of Chemistry and Biochemistry, Univ. of California, Santa Barbara

Session J32. Protein Dynamics: Ion Channels and Protein-Ligand Interactions.

Tuesday afternoon, 14:30, 212, Indiana Convention Center

14:30 J32.001 Computer Simulations of Proton Channels
Gregory A. Voth (Dept. of Chemistry and Henry Eyring Center for Theoretical Chemistry, Univ. of Utah)

15:06 J32.002 Microfabricated Patch Clamp Electrodes for Improved Ion Channel Protein Measurements
James Klemic (Departments of Applied Physics and Electrical Engineering, Yale Univ.), Kathryn Klemic (Dept. of Cellular and Molecular Physiology, Yale Univ. School of Medicine), Mark Reed (Departments of Applied Physics and Electrical Engineering, Yale Univ.), Frederick Sigworth (Dept. of Cellular and Molecular Physiology, Yale Univ. School of Medicine)

15:18 J32.003 Exchange Kinetics of a Hydrophobic Ligand Binding Protein
Jeff Vaughn, Martin Stone (Dept. of Chemistry, Indiana University, Bloomington, IN)

15:30 J32.004 Exploration of the Energy Landscape of Acetylcholinesterase by Molecular Dynamics Simulation.
J. Andrew McCammon (Howard Hughes Medical Institute, UCSD)

16:06 J32.005 Single-Molecule Probing the Energy Landscape of Enzymatic Reaction and Non-Covalent Interactions
H. Peter Lu, Dehong Hu, Yu Chen, Erich R. Vorpagel (PNNL, P.O.Box 999, Richland, WA 99352)

16:18 J32.006 Enzyme specificity under dynamic control
Nobuyuki Ota, David A. Agard (HHMI and UCSF)

16:30 J32.007 Structure and dynamics of the pore region of the nicotinic acetylcholine receptor ion channel: A molecular dynamics simulation study
Leonor Saiz, Michael L. Klein (University of Pennsylvania)

16:42 J32.008 Genetically-encoded Reporters
Ehud Isacoff (Professor of Neurobiology, University of California, Berkeley)

Session L32. Protein Dynamics:Quantum Dynamics and Transport.

Wednesday morning, 08:00, 212, Indiana Convention Center

08:00 L32.001 Quantum Mechanical Studies of Protein Dynamics and Functions
Weitao Yang (Duke University)

08:36 L32.002 Investigation of DNA through coupling molecular dynamics and electronic-structure methods.
James P. Lewis (Dept. of Physics and Astronomy, Brigham Young Univ.), Hao Wang, Otto F. Sankey (Arizona State Univ.), Eugene Starikow (Free Univ. of Berlin), Thomas E. Cheatham (Univ. of Utah)

08:48 L32.003 Electronic Properties of Overstretched DNA
Paul Maragakis, Ryan Barnett, Efthimios Kaxiras (Harvard University), Marcus Elstner, Thomas Frauenheim (University of Paderborn)

09:00 L32.004 Adiabatic Charge Dynamics in Molecules Dissolved in A Polar Solvent. Application to Charge Migration in DNA, A. L. Burin, Yu. A. Berlin, I. Kurnikov, M. A. Ratner (Dept. of Chemistry, Northwestern University, Evanston, IL 60208)

09:12 L32.005 Structural accommodation and competition in and near B-DNA oligomers.
Charles Cleveland, Robert Barnett, Uzi Landman (School of Physics, Georgia Inst. of Technology, Atlanta, GA 30032)

09:24 L32.006 Protein dynamics controlling electron tunneling routes. Going beyond the Pathways Model
Jose Onuchic (Department of Physics, University of California at San Diego, La Jolla, CA 92093-0319)

10:00 L32.007 Kinetics Probes of Protein Folding Processes
Jay Winkler, Jennifer Lee, Julia Lyubovitsky, Akif Tezcan, Harry Gray (Beckman Institute, California Institute of Technology)

10:12 L32.008 Symmetry and electron transfer in biomolecules
Maria R. D'Orsogna, Robijn Bruinsma (UCLA)

10:24 L32.009 Unusual energy transfer and structures in guanine oligodeoxynucleotides
Steven Paul Davis, Tiffany Truss, Thomas M. Nordlund (Dept. of Physics, Univ. of Alabama Birmingham)

10:36 L32.010 Diffusion-influenced reactions of polymeric reactants
Pyeong Jun Park, Sangyoub Lee (School of Chemistry and Molecular Engineering and Center for Molecular Catalysis, Seoul National University, Seoul, 151-747, Korea)

Session M32. Protein Dynamics: Longtime Dynamics.
Wednesday morning, 11:00, 212, Indiana Convention Center

11:00 M32.001 All atom long time peptide dynamics and protein folding
Karl F. Freed (University of Chicago)

11:36 M32.002 Dynamics in the unfolded state: loop closure kinetics in peptides
In-Chul Yeh, Gerhard Hummer (Laboratory of Chemical Physics, NIDDK, National Institutes of Health, Bethesda, MD 20892)

11:48 M32.003 An efficient implementation of the block normal mode approach for large proteins
Guohui Li, Qiang Cui (Dept. of Chem. University of Wisconsin, Madison)

12:00 M32.004 Long-time Langevin dynamics of cytochrome c with Go-potentials
Burak Erman (Sabanci University, Faculty of Engineering and Natural Sciences, Orhanli, 81474, Istanbul, Turkey)

12:12 M32.005 Protein Motions and Folding Investigated by NMR Spectroscopy
Arthur Palmer (Dept. of Biochemistry and Molecular Biophysics, Columbia Univ., New York, NY 10032)

12:48 M32.006 Conformational dynamics of poly-ubiquitin chains in solution
Ranjani Varadan, David Fushman (Center of Biomol. Structure amp; Organization, Dept. of Chemistry and Biochemistry, U. Maryland, College Park, MD 20742)

13:00 M32.007 Characterization of the overall and local dynamics in a protein with intermediate rotational anisotropy: Protein G as a primer, Jennifer Hall, David Fushman (Center of Biomol. Structure and Organization, Dept. Chemistry and Biochemistry, U. Maryland, College Park)

13:12 M32.008 Combined molecular dynamics and neutron scattering study of alpha-lactalbumin
M. Tarek (University of Pennsylvania and NIST Center for Neutron Research), D. A. Neumann (NIST Center for Neutron Research, Gaithersburg, MD), D. J. Tobias (Univ. of California at Irvine, Irvine, CA)

13:24 M32.009 Statistical Mechanics of double-helical polymers
Tanniemola Liverpool (Blackett Laboratory, Imperial College, London SW7 2BZ, U.K.), Alvise De Col (ETH Hoenggerber, CH-8093 Zuerich , Switzerland)

Suppl. M32.010 The worm turns: The helix/coil transition on the worm-like chain
Alex Levine, G.H. Fredrickson (Department of Chemical Engineering and the MRL, UCSB)

Session Q32. Protein Dynamics: Folding.
Wednesday afternoon, 14:30, 212, Indiana Convention Center

14:30 Q32.001 Protein folding: Mechanism, thermodynamics and dynamics
Charles L. Brooks III (The Scripps Research Institute)

15:06 Q32.002 Prediction of Protein Structure by Ab Initio Global Optimization of Potential Energy
Harold Scheraga, Adam Liwo, Jarek Pillardy, Czarek Czaplewski, Jooyoung Lee, Daniel Ripoll, Rajmund Kazmierkiewicz, Stanislaw Oldziej, Yelena Arnautova, William Wedemeyer, Jeff Saunders (Cornell Univ.)

15:30 Q32.003 Protein folding rates and pathways based on native state topology
Thomas Weikl, Ken Dill (University of California, San Francisco)

15:42 Q32.004 Peptide Folding: Many Routes to the Native State.
Adrian Roitberg (Department of Chemistry and Quantum Theory Project, University of Florida.), Carlos Simmerling (Department of Chemistry, SUNY, Stony Brook)

15:54 Q32.005 Changing protein backbone topology: Structural and dynamic consequences of the backbone cyclization in SH3 domain, Frank Schumann, Ranjani Varadan, Praveen Pudiavettil (Dept. Chem. & Biochem., U. Maryland, College Park), Julio Camarero (Lawrence Livermore National Lab), David Fushman (Dept. Chem. and Biochem., U. Maryland, College Park)

16:06 Q32.006 Dynamics and folding of individual protein molecules trapped in lipid vesicles
Gilad Haran (Chemical Physics Department, Weizmann Institute of Science, Rehovot 76100 Israel)

16:42 Q32.007 Thermal unfolding and refolding properties of the membrane protein bacteriorhodopsin under controlled perturbations using FT-IR spectroscopy
Colin D. Heyes, Jianping Wang, Mostafa El-Sayed (Laser Dynamics Lab, School of Chemistry and Biochemistry, Georgia Institute Of Technology, Atlanta, GA, 30332)

16:54 Q32.008 Fast collapse kinetics of folding and non-folding polypeptides, studied by laser T-jump spectroscopy
Linlin Qiu, Cherian Zachariah, Stephen J. Hagen (Physics Dept., Univ. of Florida, Gainesville FL)

Session S32. Protein Dynamics: Photo-Induced Dynamics.
Thursday morning, 08:00, 212, Indiana Convention Center

08:00 S32.001 Earle K. Plyler Prize Talk: The Dynamics of Photosynthetic Light Harvesting
Graham Fleming (University of California, Berkeley)

08:36 S32.002 Femtosecond study of initial events in the photocycle of photoactive yellow protein (PYP)
Jeongho Kim, Sungnam Park, Norbert Scherer (University of Chicago)

08:48 S32.003 Time-resolved macromolecular crystallography
Keith Moffat (Biochemistry, and Biophysical Dynamics, University of Chicago)

09:24 S32.004 Optical studies of dynamical processes in fluorescent proteins
Carl Liebig, William Dennis (Physics and Astronomy, University of Georgia, Athens, GA 30602), Sean Kirkpatrick, Rajesh Naik, Morley Stone (Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio 45433)

09:36 S32.005 Low Frequency Modes in Heme Proteins
Paul Champion, Florin Rosca, Dan Ionascu, Anand Kumar, Andrey Demidov, Xiong Ye, Florin Gruia (Department of Physics Northeastern University Boston MA 02115)

09:48 S32.006 Photoinduced cis-trans Isomerization from First Principles
Todd Martinez (University of Illinois at Urbana-Champaign)

10:24 S32.007 Photophysics and Nonadiabatic Dynamics of the Chromophore in Green Fluorescent Protein
Alessandro Toniolo, Michal Ben-Nun, Todd J. Martinez (Chemistry Dept., Univ. of Illinois, Urbana-Champaign)

10:36 S32.008 Gas Phase Photodynamics of the Photoactive Yellow Protein Chromophore trans-p-Coumaric Acid
Wendy Ryan, David Gordon, Donald Levy (University of Chicago)

General Session on Surface Science

Session S31. Surface Science.

Thursday morning, 08:00, 211, Indiana Convention Center

08:00 S31.001 Partial dissociation of water on Ru(0001)
Peter J. Feibelman (Sandia National Laboratories)

08:36 S31.002 Dynamics of ordering of SF_6 molecules on Ru(0001)
N. S. Faradzhev, D. O. Kusmierek, B. V. Yakshinskiy, T.E. Madey (Dept. of Physics and Lab. for Surface Modif., Rutgers University)

08:48 S31.003 IR Absorption Study of CO Monolayers on Graphite
D.A. Boyd, F.M. Hess, G.B. Hess (Physics Dept., Univ. of Virginia, Charlottesville, VA 22904)

09:00 S31.004 The First Layers of Amorphous Solid Water on Metal Surfaces
Micha Asscher, Yigal Lilach (Hebrew University)

09:12 S31.005 Preliminary Results of a Study of the Rutile TiO_2(110) Surface by Helium Atom Scattering
E.A. Akhadov, J. G. Skofronick, S. A. Safron, D. H. Van Winkle (Florida State University), F. A. Flaherty (Valdosta State Univesity)

09:24 S31.006 Wave packet calculations for helium scattering by a xenon monolayer
Lorena Tribe (University of Wisconsin-Richland), L. W. Bruch (University of Wisconsin-Madison)

09:36 S31.007 Ti atoms on and beneath the Sapphire(0001) surface
Claudio Verdozzi (Dept. of Physics-CSUN Northridge CA 91330), Peter A. Schultz (Sandia National Laboratories- MS 0316 Albuquerque NM 87185-0316), Ruquian Wu (Dept. of Physics and Astronomy, Univ. of California, Irvine CA 92697-4575), Arthur H. Edwards (Air Force Research Laboratory Bldg 914 Kirtland AFB, NM 87117-5776), Nicholas Kioussis (Dept. of Physics-CSUN Northridge CA 91330)

09:48 S31.008 Surface adsorption on a finite-width square lattice whose cut edges are at 45 degrees
Alain J Phares, Francis J Wunderlich (Villanova University, Department of Physics, Villanova, PA 19085)

10:00 S31.009 Molecular adsorption on structured surfaces
Markus Lischka, Axel Gross (Technische Universität München, D-85747 Garching, Germany)

10:12 S31.010 Density functional calculations of chemisorption and STM images of C_6H_n, n=4,5, and 6, on Cu(100).
M.F.G. Hedouin, R.E. Palmer (Nanoscale Physics Research Laboratory, School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham, B15 2TT, U.K.), Mats Persson (Department of Applied Physics, Chalmers/Goteborg University, S-41296 Goteborg, Sweden.), Nicolas Lorente (Laboratoire Collisions, Agregats, Reactivite, UMR 5589, IRSAMC, Universite Paul Sabatier, 118 route de Narbonne, F-31062 Toulouse cedex 4, France.)

10:24 S31.011 Oxide surface structure in a humid environment:the effect of a H_2/O_2 gas phase on RuO_2(110)
Q. Sun, K. Reuter, M. Scheffler (Fritz-Haber-Institut der MPG, Berlin (Germany)

Vibronic Chemistry in Isolated Molecules, at Surfaces and in Solution (DCP)

The breaking and making of chemical bonds involves the intricate and coordinated motion of electrons and nuclei. How vibrational motion of reactants and products relates to electronic reorganization is a forefront topic of modern chemical research, spanning topics of importance to isolated molecules in the gas-phase and to the complex environments of condensed phase. Surfaces, especially molecules at metals and semiconductors, is another important venue for chemistry where electronic interactions

are critically important. This symposium seeks to provide avenues for exchange between scientists working in all of these diverse areas.

Organizers: Martin Gruebele, Departments of Chemistry and Biophysics, University of Illinois at Urbana-Champaign, Alec M. Wodtke, Department of Chemistry and Biochemistry, University of California, Santa Barbara

Session T32. Vibronic Chemistry in the Gas Phase of Multiple Potential Energy Surfaces.

Thursday morning, 11:00, 212, Indiana Convention Center

11:00 T32.001 The Dissociation and Isomerization of High Energy Radical Isomers: Nuclear and Electronic Dynamics
L.J. Butler (The University of Chicago)

11:36 T32.002 Degenerate electronic reorientation in square molecules
Wei Qian, Allison Albrecht Ferro, Richard Treglio, David Jonas (Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309-0215)

11:48 T32.003 Non-adiabatic effects in the pseudorotational motion of triatomic molecules
Frank Hagelberg (Computational Center for Molecular Structure and Interactions, Jackson State University), Erik Deumens (Quantum Theory Project, University of Florida)

12:00 T32.004 Photochemistry via conical intersections: the phase change approach
Yehuda Haas (Dept. of Physical Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel)

12:36 T32.005 First-Principle Study of Geometry, Dissociation Energy and Isomer Energy Difference of Ozone Molecule
M. M. Aryal, D. D. Paudyal, Binod Dhakal, Sekhar Gurung (Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal), R. H. Scheicher, Junho Jeong, T. P. Das (Department of Physics, State University of New York at Albany, Albany NY)

Session U32. Vibronic Chemistry: Vibrational Influences on Electron Transfer.

Thursday afternoon, 14:30, 212, Indiana Convention Center

14:30 U32.001 Vibrationally Resolved Electron Transfer Rates in Solution
Kenneth G. Spears (Northwestern University, Chemistry Department)

15:06 U32.002 Femtosecond pump-probe photoelectron spectra of wavepackets in small molecules
Vincent McKoy (California Institute of Technology)

15:42 U32.003 Optical Control of the Electron in the Simplest Electron Transfer Reaction
Benjamin Schwartz (UCLA Dept. Chem. & Biochem.)

16:18 U32.004 Dissipative wave packet dynamics and electron transfer
Joachim Ankerhold, Andreas Lucke (Fakultaet fuer Physik, Universitaet Freiburg, Germany)

16:30 U32.005 Is the Hexaamminecobalt Electron-Exchange Reaction adiabatic or diabatic?
Daniel Cox, Robert Endres, Montiago LaBute (Department of Physics, University of California, Davis)

16:42 U32.006 Bonding charge from nonspherically distorted ions in a model with full ionic charges
L. L. Boyer, M. M. Ossowski, M. J. Mehl (Naval Research Laboratory), H. T. Stokes (Brigham Young University)

16:54 U32.007 First principle calculations of the vibrational spectrum of methane
David Schwenke (NASA Ames Research Center)

17:06 U32.008 Highly Accurate Vibrational Transition Energies and a Heat of Formation for the High Energy Density Material Tetrahedral N_4
Timothy Lee (NASA Ames Research Center), Jan Martin (Department of Organic Chemistry, Weizmann Institute of Science)

Session W32. Vibronic Chemistry at Surfaces.
Friday morning, 08:00, 212, Indiana Convention Center

08:00 W32.001 Surface Reactivity of Highly Vibrationally Excited Molecules Prepared by Pulsed Laser Excitation: CH_4 on Ni(100)
Rainer D. Beck (Ecole Polytechnique Federale de Lausanne (EPFL), Laboratoire de Chimie Physique Moleculaire, CH-1015 Lausanne, Switzerland)

08:36 W32.002 State-Resolved Dissociative Chemisorption Dynamics of Vibrationally Excited Molecules
Arthur Utz (Tufts University Department of Chemistry)

09:00 W32.003 State resolved vibrational relaxation in the scattering of H_2 and D_2 from copper and palladium surfaces
Greg Sitz, Leah Shackman (The University of Texas at Austin)

09:24 W32.004 Vibrational effects on dissociative chemisorption of hydrogen: 6D quantum dynamics results for Cu(100) and Pt(111).
Geert-Jan Kroes (Leiden Institute of Chemistry, Leiden University)

10:00 W32.005 Electron-hole pair generation in the interaction of vibrational excited and ground state molecules with metal surfaces
D.J. Auerbach (Almaden Research Center, IBM Research Division, 650 Harry Road, San Jose, CA 95120-6099), Y. Huang, M. Murphy, J. White, A.M. Wodtke (Chemistry, University of California, Santa Barbara, CA)

10:24 W32.006 Quantum States of Hydrogen on Pt (111): Ab-initio Modeling and Vibrational Measurements
Stefan Badescu, See-Chen Ying (Brown University, RI), Petri Salo, Tapio Ala-Nissila (Helsinki Univ. of Tech., Finland), Karl Jacobi, Yuemin Wang, Kolja Bedurftig, Gerhardt Ertl (Fritz-Haber Inst., Berlin)

10:36 W32.007 Hindered rotation of H_2 and D_2 adsorbed interstitially in nanotube bundles
Milen Kostov, Milton Cole (Department of Physics, Penn State University, University Park, Pennsylvania 16802)

10:48 W32.008 Dynamics of reactive scattering: Hyperthermal energy collisions of state-selected Br_2^+ on Pt(111) M. Maazouz, P. L. Maazouz, D. C. Jacobs (University of Notre Dame)

Session X32. Vibronic Chemistry: Spectroscopy of Clusters.
Friday morning, 11:00, 212, Indiana Convention Center

11:00 X32.001 Vibronic and Vibrational Bond Breaking and Making at Interfaces
Giacinto Scoles (Princeton University)

11:36 X32.002 Exciting Molecules and Clusters using the Free Electron Laser FELIX
Gert von Helden (FOM Institute Rijnhuizen, Edisonbaan 14, 3439 MN Nieuwegein, The Netherlands)

12:12 X32.003 Structural and Vibrational Coherence of Isolated and Solvated Molecules
Brooks Pate (Department of Chemistry, University of Virginia)

12:48 X32.004 Dynamics of Adsorption on Metal Surfaces Probed with Single-Molecule Resonance Raman Spectroscopy
Gilad Haran, Amir Weiss (Chemical Physics Department, Weizmann Institute of Science, Rehovot 76100,Israel)

13:00 X32.005 Laser Induced Fluorescence Studies of the State-to-state Rotational Energy Transfer Rates in Bi_2 $A(0_u^+)$, v'=1
Glen P Perram (Air Force Institute of Technology), Robert E Franklin (US Air Force Aeronautical Systems Center)

13:12 X32.006 Helium pressure broadening of HDO between 2 and 80 K
Theodore J. Ronningen, Frank C. De Lucia (The Ohio State University)

The Physical and Electronic Structure of Conjugated Polymers: From Photophysics to Devices

Conjugated polymers are remarkable materials that combine the electrical properties of semiconductors with the mechanical properties and processing advantages of plastics. As a result, these materials show great promise for use in a variety of optoelectronic applications, including LEDs, displays and photovoltaic devices. This focused session will provide a broad overview on the current state-of-the-art for what is known concerning the critical relationship between the physical properties of conjugated polymers (e.g. chain conformation and orientation) and the electronic properties of conjugated polymers (e.g. presence of interchain electronic species, behavior in optoelectronic devices). Experimental and theoretical papers are solicited on a wide variety of phenomena, including but not limited to: processing effects on conjugated polymer solutions or films, spectroscopy of conjugated polymer solutions or films, the nature of conjugated polymer interchain species, carrier recombination and transport properties in conjugated polymers, the relationship between film morphology and device performance, properties of conjugated polymer/metal interfaces, studies of single conjugated polymer molecules. Authors are encouraged to stress the relationship between their work and the applications of these materials in practical devices. Contributions span experimental, theoretical and computational methodologies.

Organizer: Benjamin J. Schwartz, Dept. of Chemistry and Biochemistry, UCLA

Session T28. Effects of Morphology on Conjugated Polymer Electronic Properties.

Thursday morning, 11:00, 208, Indiana Convention Center

11:00 T28.001 Aggregation Behavior of Dendritic Side Group Luminescent Polymers
Lewis Rothberg (University of Rochester Department of Chemistry)

11:36 T28.002 Probing the Conformation of Oligo(phenylenevinylene) Chromophores using Single Molecule Spectroscopy and Gas-Phase Ion Chromatography
A. Summers, Steven K. Buratto, John E. Bushnell, Paul R. Kemper (Department of Chemistry and Biochemistry, University of California, Santa Barbara), Matthew R. Robinson (Department of Materials, University of California, Santa Barbara), Guillermo C. Bazan, Michael T. Bowers (Department of Chemistry and Biochemistry, University of California, Santa Barbara)

11:48 T28.003 The effects of nanocrystalline domains on the photophysics of PPV and related materials
Christopher Bardeen (Department of Chemistry, University of Illinois)

12:24 T28.004 Mapping the kinetics of photo-excited states in conjugated polymers with fluorescence bleaching-recovery and time-resolved fluorescence spectroscopy
Sang-Hyun Lim, Thomas Bjorklund, Christopher Bardeen (University of Illinois)

12:36 T28.005 Non-classical light emission from single conjugated polymers
Christopher Hollars, Stephen Lane, Thomas Huser (Lawrence Livermore National Laboratory)

12:48 T28.006 Inter and intra molecular interactions in conjugated polymers and dendrimers
Ifor Samuel (School of Physics and Astronomy, University of St Andrews, St Andrews, Scotland)

13:24 T28.007 Ionomeric Control of Interchain Interactions in Conjugated Polymers
Benjamin Schwartz, Thuc-Quyen Nguyen (UCLA Dept. of Chemistry and Biochemistry)

Session U28. Improvements in Conjugated Polymer Device Design and Understanding.

Thursday afternoon, 14:30, 208, Indiana Convention Center

14:30 U28.001 Charge injection in organic semiconductors
George Malliaras (Cornell University), Department of Materials Science and Engineering Collaboration

15:06 U28.002 Exciton and exciplex confinement in light emitting polymers
Arthur J. Epstein (The Ohio State University, Columbus, OH 43210)

15:42 U28.003 Charge Transport at Low Electric Fields in π-Conjugated Polymers
Gytis Juska, Kristijonas Genevicius, Kestutis Arlauskas (Dept. of Solid State Electronics, Vilnius University, Sauletekio 9, LT-2040, Vilnius, Lithuania), Ronald österbacka, Henrik Stubb (Dept. of Physics, Åbo Akademi University, Porthansgatan 3, FIN-20500 Turku, Finland)

15:54 U28.004 Charge Separation and Recombination Dynamics in Donor/Acceptor Semiconductor Polymers for Photovoltaic Applications
Carlos Silva (University of Cambridge)

16:30 U28.005 Dependence of Picosecond Fluorescence Dynamics on Chemical Structure and Temperature in Conjugated Polymers
Thomas Bjorklund, Sang-Hyun Lim, Christopher Bardeen (University of Illinois)

16:42 U28.006 Self-Diffusion in Polymerized Microemulsions Using Pulsed-Gradient NMR
S. Chandran, E. von Meerwall, K. Fletcher, J. Slivka, J. Kuminski, S. Lopina, M. Cheung (Univ. of Akron)

16:54 U28.007 Modeling of the specific binding of biomolecules by molecularly imprinted polymeric gels.
David B. Henthorn, Kinam Park, Nicholas A. Peppas (NSF IGERT Center on Therapeutic and Diagnostic Devices, School of Chemical Engineering, Dept. of Industrial and Physical Pharmacy, Dept. of Biomedical Engineering, Purdue University, West Lafayette, IN, USA)

Session W28. Advances in the Electronic Structure of Conjugated Polymers.

Friday morning, 08:00, 208, Indiana Convention Center

08:00 W28.001 Quantum Chemical Models of the Photophysics of Organic Semiconductors: Effective Particles and Energy Landscapes
D. Yaron (Department of Chemistry, Carnegie Mellon)

08:36 W28.002 Effects of charge transfer, wind force, asymmetry, and gating on electron transport in molecular films
P.E. Kornilovitch, A.M. Bratkovsky (Hewlett-Packard Laboratories, Palo Alto, CA)

08:48 W28.003 Modeling the Effects of Structural and Environmental Disorder on the Electroabsorption Spectra of MEH-PPV
L. Angela Liu, D. Yaron, S. Wachsmann-Hogiu, D. Lam, L.A. Peteanu (Department of Chemistry, Carnegie Mellon)

09:00 W28.004 Excited state dynamics in molecule electronic devices: the role of relaxation and decoherence
Eric Bittner (Univ. of Houston)

09:36 W28.005 Energy Excitation Transfer in a Single Molecule of Poly(p-phenylene vinylene)
Gil Claudio, Eric Bittner (Department of Chemistry, University of Houston)

09:48 W28.006 Theoretical Investigation of Phase Transitions and Deterioration of the Electro-Optic Coefficient in Chromophore-Polymer Materials
Oleg Prezhdo, Yuriy Pereverzev (Department of Chemistry, University of Washington, Seattle WA, 98195-1700)

10:12 W28.007 Mechanically Tuning the Color of Polyacetylene
Daniel P. Aalberts, Benjamin K. Cooper (Williams College)

Suppl. W28.008 Variable Range Hopping in Low Dimensions.
Vladimir Prigodin (The Ohio State University), Joo Jinsoo (Korea Univeristy), Epstein Arthur (The Ohio State University)

Session X28. Advances in Conjugated Polymer Materials Design and Understanding.

Friday morning, 11:00, 208, Indiana Convention Center

11:00 X28.001 n-Type conjugated polymers: advances in synthesis, photophysics, charge transport, and device applications
Samson A. Jenekhe (University of Washington)

11:36 X28.002 Enhanced performance in polymer light emitting-diodes using polybenzobisazoles as electron transport materials
Maksudul m. Alam, Samson A. Jenekhe (Departments of Chemical Engineering and of Chemistry, University of Washington, Box 351750, Seattle, WA 98195-1750)

11:48 X28.003 Structure/Property Relationships in Polymer Light-emitting Diodes
Mary Galvin (Materials Science and Engineering, University of Delaware)

12:24 X28.004 Energy Transfer Dynamics in Light-Harvesting Dendrimers
Joseph S. Melinger (ESTD Naval Research Laboratory Washington DC 20375), Dale Mc Morrow (ESTD Naval Research Laboratory Washington DC 20375), Valeria D. Kleiman (Dept. of Chemistry University of Florida Gainesville Fl 32611-7200)

12:36 X28.005 Microenvironmental and structural effects on photophysical properties of substituted organic semiconductors
Sebastian Wachsmann-Hogiu, Danny Lam, Arindam Chowdhury, Linda Peteanu, Angela Liu, David Yaron (Dept. of Chemistry, Carnegie Mellon Univ., Pittsburgh, PA 15213)

12:48 X28.006 Near-field Scanning Optical Microscopy of Polyfluorene Thin Films
David Vanden Bout (Texas Materials Institute and Center for Nano and Molecular Materials Science and Technology & Department of Chemistry & Biochemistry, University of Texas at Austin)

13:24 X28.007 Torsional Motion in the Photophysics of Poly(p-phenyleneethynylene)s
Mikail Sluch, Uwe Bunz, Mark Berg (Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC 29208), Adelheidt Godt (Max-Plank-Institut für Polymerforschung, Mainz, Germany)

Suppl. X28.008 Electrical Transport of Long DNA Molecules on Liuid-Solid Interfaces
Vladimir Samuilov, Young-Soo Seo, Jonathan Sokolov, Miriam Rafailovich (Department of Materials Science, SUNY at Stony Brook), Benjamin Chu (Department of Chemistry, SUNY at Stony Brook)

Physics of Chemically Modified Interfaces (DCP/DMP)

Chemical modification of interfaces is a means to many ends including molecular electronics, ultrathin gate dielectrics, tribology. Recently, there has been considerable effort to use the methods of synthetic chemistry to modify the properties of interfaces, leading to the creation of new systems and the observation of novel physical phenomena. Our goal is to foster interactions and exchange between members of this diverse community, as well as between theorists and experimentalists. Experimental and theoretical papers in all areas related to physics of chemically modified interfaces are included, such as:

Novel probes of chemically modified interfaces

Dynamics of charges at chemically modified interfaces

Electron transmission through chemically modified interfaces

Devices based on chemically modified interfaces

Nanostructured chemically modified interfaces

Chemically modified nanoparticle interfaces
Biological surfaces

Organizer: Eric Borguet, Dept. of Chemistry & Surface Science Center, Univ. of Pittsburgh

Session T31. Tribology of Chemically Modified Interfaces.
Thursday morning, 11:00, 211, Indiana Convention Center

11:00 T31.001 Effect of surface modification on smooth and stick-slip sliding
Jacob Israelachvili (University of California, Santa Barbara 93106)

11:36 T31.002 Nanotribology of a Vapor Phase Lubricant: A Quartz Crystal Microbalance Study of Tricresylphosphate (TCP) Reactive Films on Iron and Chrome
Cherno Jaye, Mohammed Abdelmaksoud, Jonathan Bender, Jacqueline Krim (Dept. of Physics, North Carolina State University)

11:48 T31.003 Friction Measurement on Organic Monolayers Formed by Nanografting
Ying Hu, Giacinto Scoles, Kyle Vanderlick (Princeton Materials Institute), Gang-yu Liu, William Price (University of California at Davis), Milan Mrksich (University of Chicago)

12:00 T31.004 Squeezing molecular thin lubrication films
B.N.J. Persson (IFF, FZ Juelich, D-52425 Juelich, Germany)

12:36 T31.005 ADHESION AND FRICTION OF POLYMER SURFACES
Nianhuan Chen (University of California, Santa Barbara 93106), Nobuo Maeda, Matthew Tirrell, Jacob Israelachvili (UCSB)

12:48 T31.006 Tuning the Binding Energy: Electrochemical Control of Molecular Self-Assembly
Yufan He, Tao Ye, Eric Borguet (Surface Science Center, University of Pittsburgh)

13:00 T31.007 Kinetics and dynamics of the desorption of oligomeric lubricants
Andrew Gellman (Carnegie Mellon University)

13:36 T31.008 Thermal Desorption of Large Molecules from Solid Surfaces
Kristen Fichthorn, Radu Miron, Ashish Kulkarni (The Pennsylvania State University)

13:48 T31.009 Strain dependence of surface diffusion of Co on Pt surface.
Renat Sabiryanov, Kyeongjae Cho, Bruce Clemens, William Nix, Stanford University Team

Session U31. Physics of Chemically Modified Semiconductor Surfaces I.
Thursday afternoon, 14:30, 211, Indiana Convention Center

14:30 U31.001 Surface-Related Phenomena in MEMS
Roya Maboudian (Department of Chemical Engineering, University of California at Berkeley)

15:06 U31.002 Band bending and electrical transport at chemically modified silicon surfaces
Greg Lopinski, Tim Ward, Oleksa Hul'ko, Rabah Boukherroub (Steacie Institute for Molecular Sciences, National Research Council Canada), Molecular Interfaces Program Team

15:18 U31.003 Controlling metallic contacts to self-assembled monolayers and molecular electronic devices
Amy Walker, Tim Tighe, Orlando Cabarcos, Mike Reinard, Brendan Haynie, David Allara, Nick Winograd (Pennsylvania State University)

15:30 U31.004 Using Organonitriles to Modify the Semiconductor Interface
Michael A. Filler, Stacey F. Bent (Stanford University, Department of Chemical Engineering)

15:42 U31.005 A Molecular Dynamics Study of the Alignment of Silver Nano-Clusters on H-terminated Si(111)
Y. F. Shi, B. Q. Li, J. M. Zuo (Department of Materials Science and Engineering and Materials Research Laboratory, Univ. of Illinois at Urbana and Champaign, Urbana, Illinois 61801)

15:54 U31.006 Novel Reactions of Organic Molecules for Controlled Modification of Semiconductor Surfaces
Doug Doren (University of Delaware)

16:30 U31.007 Origin of low sticking of cyclopentene on the diamond(001) surface

Leonard Kleinman, Jun-Hyung Cho (University of Texas at Austin)

16:42 U31.008 Incorporation of hyperthermal energy oxygen ions into silicon oxide thin films: Comparative study of O^+ vs. O_2^+ reactivities.
Tochko Tzvetkov, Xiangdong Qin, Dennis C. Jacobs (University of Notre Dame)

16:54 U31.009 Organic Monolayers on Silicon and Germanium Surfaces: Harnessing Synthetic Versatility toward Intelligent Interfacial Design
Jr. Porter, J. M. Schmeltzer, Jillian M. Buriak (Department of Chemistry, Purdue University, 1393 Brown Labs of Chemistry, West Lafayette, IN 47907)

17:06 U31.010 Grazing-Incidence Diffraction Study of Langmuir Films of Amphiphilic Monodendrons
W.-J. Pao, F. Zhang, P.A. Heiney (Dept. of Physics and Astronomy and Laboratory for Research on the Structure of Matter, Univ. of Pennsylvania), W.-D. Cho, C. Mitchell, V.K. Balagurusamy, V. Percec (Dept. of Chemistry and Laboratory for Research on the Structure of Matter, Univ. of Pennsylvania)

17:18 U31.011 Molecular Packing of Amiphiphiles with Crown Polar Heads at the Air-Water Interface
K. Larson (Dept. of Materials Science and Engineering, Iowa State University, Ames, IA), D. Vaknin (Ames Laboratory and Dept. of Physics and Astronomy, ISU), O. Villavicencio, D. McGrath (Dept. of Chemistry, Univ. of Arizona, Tucson), V. V. Tsukruk (Dept. of Materials Science and Engineering, ISU)

Session W31. Physics of Chemically Modified Semiconductor Surfaces II.

Friday morning, 08:00, 211, Indiana Convention Center

08:00 W31.001 Nonlinear Optical Characterization of Polymer Surfaces.
Y. R. Shen (University of California at Berkeley)

08:36 W31.002 Separating Bulk and Surface Contributions to the Second Order Nonlinear Optical Response of Chemically-Modified Semiconductor (Germanium) Interfaces
V. Fomenko, D. Bodlaki, E. Borguet (Univ. of Pittsburgh, Dept. of Chemistry, Pittsburgh, PA 15260)

08:48 W31.003 Nanoscale Fabrication and Electronic Characterization of Chemically Modified Silicon Surfaces Using Conductive Atomic Force Microscopy in Liquids
Matthew Such, Reagan Kinser, Cinthia Herrera, Mark Hersam (Materials Sci. and Eng., Northwestern)

09:00 W31.004 Surfaces of Microparticles in Colloids: Structure and Molecular Adsorption Kinetics
Hai-Lung Dai (Department of Chemistry, Univiersity of Pennsylvania, Philadelphia, PA 19104-6323)

09:24 W31.005 Optical second-harmonic spectroscopy of chemically-modified silicon and silicon-dioxide surfaces
M.C. Downer, Y.Y. Jiang, D. Lim (University of Texas at Austin), Dept. of Physics Collaboration

09:36 W31.006 Thermodynamic Stability of High-K Dielectric Metal Oxides ZrO_2 and HfO_2 in Contact with Si and SiO_2
Maciej Gutowski, John E. Jaffe (Theory, Modeling & Simulation, PNNL, P.O. Box 999, Richland, WA 99352), Chun-Li Liu, Matt Stoker (Advanced Process Development and External Research Laboratory, Motorola, Mesa, AZ 85202), Rama I. Hegde, Raghaw S. Rai, Philip J. Tobin (Advanced Process Development and External Research Laboratory, Motorola, Austin, TX 78721)

09:48 W31.007 Structure at Polymer/Water Interface
Hasnain Rangwalla, Keshav Gautam, Ali Dhinojwala (Department of Polymer Science, The University of Akron), Shawn Dougal, Mohsen Yeganeh (ExxonMobil Corporate Strategic Research Laboratories, NJ)

10:00 W31.008 Dry layer formation? Solvent polarity at hydrophobic solid-liquid surfaces
Robert Walker (Department of Chemistry, University of Maryland), Xiaoyi Zhang (Chemical Physics Program, University of Maryland), Okan Esenturk (Department of Chemistry, University of Maryland)

10:12 W31.009 Surface Vibrational Spectroscopy on Nylons
Seok-Cheol Hong, Chun Zhang, Y. R. Shen (Department of Physics, University of California, Berkeley)

10:24 W31.010 Nonlinear spectroscopy at the electrochemical interface
Philippe Guyot-Sionnest (James Franck Institute, The University of Chicago, Chicago, IL 60637)

Session X31. Electron Transmission through Chemically Modified Interfaces.

Friday morning, 11:00, 211, Indiana Convention Center

11:00 X31.001 Electrical and Electronic Properties of Chemically Modified Silicon Surfaces
Nathan Lewis (California Institute of Technology)

11:36 X31.002 Tunneling Through Novel Ultrathin Dielectrics for Semiconductor Interfaces Probed by Second Harmonic Generation
Eric Borguet, Dora Bodlaki, Vasiliy Fomenko (Surface Science Center, University of Pittsburgh)

11:48 X31.003 Charge transfer at metal/solid polymer interfaces in the presence of liquids
Joe Wasem, Steve Langford, Tom Dickinson (Washington State University)

12:00 X31.004 Surface Phenomena and Chemical Functionalization of Carbon Nanotubes: Implications to Molecular Electronics and Bioelectronics
Moonsub Shim, Robert Chen, Nadine Wong Shi Kam, Hongjie Dai (Stanford Univ., Dept. of Chem.)

12:12 X31.005 Mechanistic Studies of Electron Tunneling through Organic Monolayer Films
David Waldeck (University of Pittsburgh)

12:48 X31.006 Electron transport through CH_3- and CF_3- Terminated Alkanethiol Monolayers on Au(111) Studied by Scanning Tunneling Microscopy.
J. PfLAUM (Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544), Jr. Colorado, O.E. Shmakova, T.R. Lee (Dept. of Chemistry, Univ. of Houston, Texas 77204-5641), S. Scandolo, G. Scoles, A. Kahn (Princeton Materials Inst., Princeton Univ., Princeton, NJ 08544)

13:00 X31.007 MD simulations of water between plates
Subramanian Vaitheeswaran (Dept. of Physics, University of Maine), Jayendran C. Rasaiah (Dept. of Chemistry, University of Maine)

13:12 X31.008 Structural determination of monolayer p-phenylene oligomer films on GRAFOIL
E.J. Kintzel Jr. (MARTECH and the Department of Physics, Florida State University), S. Rols, K.W. Herwig (Oak Ridge National Laboratory, Oak Ridge, TN)

13:24 X31.009 Surface energy calculations within the free electron model.
A.J. Arko, T. Durakiewicz, J.J. Joyce, M.T. Butterfield, D.P. Moore (Los Alamos National Laboratory, Los Alamos, NM 87545), S. Halas (UMCS Lublin, Poland)

13:36 X31.010 Surprising Electronic-Magnetic Properties of Close Packed Organized Organic Layers-Magnetization of Chiral Monolayers of Polypeptide
Ron Naaman, Itai Carmeli, Viera Skakalova (Dep. of Chemical Physics, Weizmann Institute, Rehovot, Israel), Zeev Vager (Dept. of Particle Physics, Weizmann Institute, Rehovot, Israel)

13:48 X31.011 Influence of humidity on light emission from gold films in an STM
D George Walmsley, Paul Dawson, Joe O'Mahony (Department of Pure and Applied Physics, Queen's University, Belfast BT7 1NN)

New Techniques, Applications and Instruments in X-Ray Absorption Spectroscopy (DCP/GIMS)

X-ray absorption spectroscopy (XAS) has been instrumental to the advancement of many fields, including biology, chemistry, physics, and materials science. Recent developments in XAS have enabled researchers in these fields to investigate phenomena that would otherwise be impossible to study. This call-for-abstracts solicits reports in all areas related to new developments in both experimental and theoretical aspects of x-ray absorption spectroscopy. Results on x-ray absorption near edge spectroscopy or extended x-ray absorption fine structure investigations of nanoparticles, improved multiple

scattering theories, new ultrafast x-ray sources and time-resolved absorption techniques and applications, and the high spatial resolution x-ray microscopy are particularly encouraged. This symposium draws attention to the combined strength of new technologies and new theories, and is sponsored by both the Division of Chemical Physics (DCP) and the Instrumentation and Measurement Science Topical Group (GIMS).

Organizers: Ting Guo, Chemistry Department, University of California, Davis, CA 95616
Robert Schoenlein, Materials Sciences Division, Lawrence Berkeley National Laboratory Berkeley, CA 94720, John Rehr, Department of Physics, University of Washington

Session W13. New Techniques, Applications and Instruments in X-Ray Absorption Spectroscopy: I.

Friday morning, 08:00, 106, Indiana Convention Center

08:00 W13.001 Progress in the Theory and Interpretation of X-Ray Absorption Spectra
J. J. Rehr (Dept. of Physics, Univ. of Washington)

08:36 W13.002 Resonant Inelastic Soft-x-ray Scattering (RIXS) in Probe of Electronic Structure of Matter
Jinghua Guo (Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720)

08:48 W13.003 X-ray fluorescence holography--some recent developments
Stefano Marchesini (LBNL), Norman Mannella, Charles S. Fadley, Michel Van Hove (LBNL, UCDavis), Wayne C Stolte (U. Nevada), Jerome J Bucher, Lorenzo Fabris, Mark W West, Michael J Press, Zahid Hussain (LBNL)

09:00 W13.004 Imaging Magnetic Structures by means of X-ray Microscopy and Coherent Scattering
Joachim Stöhr (Stanford Synchrotron Radiation Laboratory)

09:36 W13.005 EXAFS of Materials with Multiple Absorbing Sites
Scott Calvin, Roman Izaac, Mihail Rivlin, M. L. denBoer (Hunter College of the City University of NY)

09:48 W13.006 Chemical Speciation via X-ray Emission Spectra
A.L. Ankudinov, J.J. Rehr, W.T. Elam (U. of Washington), J.R. Sieber (NIST)

10:00 W13.007 First Principle Calculations of X-ray Absorption of Complex Systems
Yi Luo (Theoretical Chemistry, Royal Institute of Technology, SCFAB, S-10691 Stockholm, Sweden)

10:12 W13.008 Micro-XAFS study of Tc and Mn in bioreduced Hanford sediments
S. M. Heald, J. P. McKinley, J. M. Zachara (PNNL, Richland WA)

10:24 W13.009 The Unusual Valence Behaviour of Eu in $[EuP_5W_{30}O_{110}]^{12-}$
L. Soderholm, M. R. Antonio, C. W. Williams, S. Skanthakumar (Chemistry Division, Argonne National Laboratory, Argonne, IL 60439.)

Session X13. New Techniques, Applications, and Instruments in X-Ray Absorption Spectroscopy: II.

Friday morning, 11:00, 106, Indiana Convention Center

11:00 X13.001 Time-Resolved X-Ray Scattering from Excited Materials
R.W. Falcone (University of California, Berkeley)

11:36 X13.002 Ultrafast lasers and x-ray sources for x-ray absorption spectroscopy in chemical research
Christoph Rose-Petruck (Department of Chemistry, Box H, Brown University, Providence RI 02912)

11:48 X13.003 Properties of Liquid Silicon and Carbon Studied by Ultrafast Time-Resolved X-Ray Absorption Spectroscopy

Steven Johnson, Aaron Lindenberg, Andrew MacPhee, Roger Falcone (UC Berkeley), Phillip Heimann (Advanced Light Source, LBNL), Harald Jeschke, Martin Garcia (Freie Universität Berlin), John Rehr (UW Seattle), Dick Lee (LLNL), Zenghu Chang (Kansas State University)

12:00 X13.004 Ultrafast time resolved X-ray diffraction and EXAFS studies of transient structures in liquids and solids
Dmitri A. Oulianov, Ivan V. Tomov, Peter M. Rentzepis (Department of Chemistry, University of California, Irvine, CA 92697)

12:24 X13.005 Soft X-ray Absorption Spectroscopy of Single Nanocrystals
A. Paul Alivisatos (University of California, Berkeley)

13:00 X13.006 Surface Segregation of Ni/Co Bimetallic Nanoparticles Produced in Single-Walled Carbon Nanotube Synthesis
Guangjun Cheng Ting Guo (University of California at Davis),

13:12 X13.007 Investigating the Local Electronic Structure of Vacancy Ordered Perovskite Oxides
E. Hammas, R.F. Klie, N.D. Browning (University of Illinois at Chicago, Department of Physics, 845 West Taylor Street, Chicago, IL 60607. USA.)

13:24 X13.008 Occupied and unoccupied electronic structure of DNA polynucleotides: PES and XAS study
Masashi Furukawa (RIKEN amp; ISIR, Osaka Univ.), Tomoyuki Takeuchi (ISSP, Univ. of Tokyo), Hiroyuki S. Kato, Tadahiro Komeda, Maki Kawai (RIKEN), Tomoji Kawai (ISIR, Osaka Univ.), Shik Shin (ISSP, Univ. of Tokyo amp; RIKEN)

13:36 X13.009 Photoexcited State Molecular Structures in Solution Studied by Pump-Probe XAFS
Lin Chen (Chemistry Division, Argonne National Laboratory)

13:48 X13.010 Future XUV sources from Ultrafast Laser Technology
Enam Chowdhury, Barry Walker (University of Delaware)

Division of Chemical Physics Poster Session (in Poster Session III.)

Tuesday afternoon, 14:00, Exhibit Hall D, Indiana Convention Center