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# Materials and Molecular Research Division

## Newsletter

Lawrence Berkeley Laboratory  
Berkeley, California

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September 1979  
Volume 3, No. 9

### RESEARCH PROFILE

#### PREDICTIVE CHEMICAL MODELS FOR NEW ENERGY PROCESSES

*Leo Brewer*

Although my research has ranged from study of gases of astronomical interest and energy-important high-temperature refractory materials to metal alloys of superconducting interest at liquid hydrogen temperatures, the common thread has been the combination of theory with experiment to develop predictive models that would provide practical values of the properties of a wide range of materials up to very high temperatures. I began my research in organic chemistry as an undergraduate at Cal Tech under the direction of Professor Howard Lucas. At the advice of Professor Linus Pauling, chairman of the Chemistry Department at Cal Tech, I went to Berkeley in Fall 1940 to continue my research under the direction of Professor Axel Olson.

#### MANHATTAN PROJECT

I completed my Ph.D. thesis in late 1942, and took a post-doctoral position with Professors Wendell Latimer and Ermon Eastman in order to work on the Manhattan Project at Berkeley. I was told about the discovery of the new element plutonium, and the concern about the properties of the metal,

(continued on page 4)



**SANDRA STEWART GETS 15-YEAR PIN**

"She began as a purchasing clerk and rose to be a key member of the MMRD support staff," remarked DAVE SHIRLEY addressing a group of fellow employees gathered to celebrate and recognize fifteen years of work at the Laboratory by SANDRA STEWART. DAVE continued, "It is a tribute to the skill and ability SANDY possesses, that most purchases for the Division are received on time in spite of the bureaucracy of both LBL and DOE."

SANDY started with LBL in the Purchasing Department in 1964, but moved to MMRD (then IMRD) within a year and has been with our Division since that time. SANDY, in fact, worked

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## STEWART (Continued)

briefly for the Division on campus and was the first group of permanent people to move into Bldg 62 when it was completed.

SANDY indicates that working with people, interaction on an individual basis plus the ability to be able to help when purchasing problems arise are the most satisfying aspects of her job. And these aspects have grown with the assistance of CONWAY PETERSON. "He always encouraged job growth by delegation of duties and responsibilities," SANDY says.

But away from the job, who is this person, SANDRA STEWART?

Well, she's a Trekkie of long standing as well as a photographer of skill and imagination with a persistent interest in pre-history and a desire to bring these two interests together by becoming an expert in archeological photography. Toward this end she is also a student in anthropology at the College of Alameda.

SANDY says she didn't hire on back in 1964 as a career person - but time and opportunity and personal growth continued so she stuck around until now it has been fifteen years! Congratulations, SANDY.

## ELLIPSOMETRY CONFERENCE

The Fourth International Conference on Ellipsometry was held at LBL, August 20-22, 1979, under the joint sponsorship of MMRD/LBL and the Army Research Office.

Ellipsometry is an experimental technique for the study of surfaces and thin films by the reflection of polarized light. Measurements are extraordinarily sensitive and can be conducted in any optically transparent medium.

The principal Conference topics were covered by five invited speakers and 35 additional papers on topics of Optical Theory, Instrumentation and Techniques, and Applications. The Conference drew 103 participants with some 37 of these coming from 14 foreign countries.

The Conference, part of an on-going series initiated in 1963 at NBS in Washington, D.C. and continued at the University of Nebraska in 1968 and 1975, was to provide an interdisciplinary forum to determine the present status of the field of ellipsometry, to bring into focus new experimental and theoretical developments, and to explore new applications.

Many new researchers have entered the field and steady progress is being made on the theoretical optical problems of rough surfaces, atomic coverage, and inhomogeneous materials. Applications of the technique have been broadened and now include the study of multilayer electrochemical films, corrosion under organic coatings, ion-implanted and laser-annealed surfaces, and glassy metal/semiconductor interfacial regions. In addition, the great sensitivity of ellipsometry for the measurement of submonomolecular layers continues to be utilized for absorption studies in ultrahigh vacuum.

Striking progress was reported in some medical applications in which the action of enzymes and antibodies on protein layers is measured by following thickness changes of the protein.

The use of spectroscopic ellipsometry, which was at its beginning at the last conference, is probably the most important advance that has since occurred. Questions of interest pursued by such measurements include the electronic structure of surface regions and how it is affected by very thin surface layers, identification of reaction products and intermediates.

Instrumentation developments are aimed at further increasing speed and

## ELLIPSOMETRY CONFERENCE (Continued)

precision of measurements, particularly for spectral work. Papers attracting special interest at the Conference concerned the use of a stabilized transverse Zeeman laser as a light source of rapidly varying state of polarization, and the application of photon counting. The simultaneous measurement of reflectance has also been further explored. It can be expected that, in addition, partial polarization will be measured in the future. With the determination of all four Stokes parameters, the experimental information will be greatly increased.

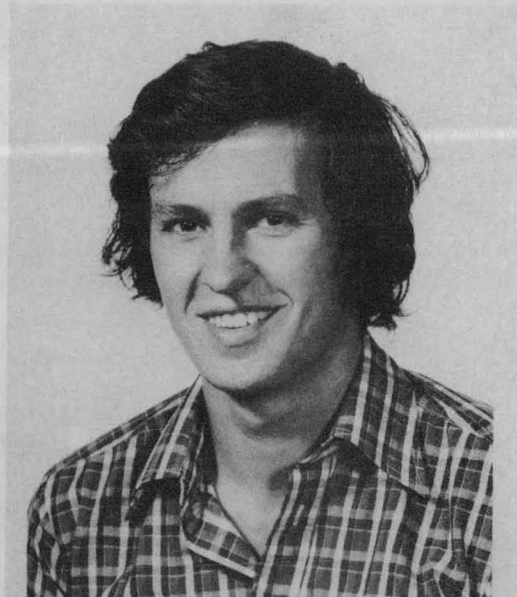
The organizing committee for the Conference was composed of D. E. Aspnes of Bell Labs, R. M. A. Azzam of the University of Nebraska, and R. M. MULLER of MMRD.

The successful operation of the technical aspects of the Conference was in large measure due to the personal help of CONWAY PETERSON. Thanks also go to FELIX SCHWAGER, WALTER GIBA, MARGIE JANZEN, ETHYL SKRYDLINSKI, SUSAN QUARELLO, CORRINE COUGHANOWR, JOE FARMER, JIM FALTEMIER, Loretta Lizama and Peggy Little.

Three manufacturers of ellipsometers and optical components made contributions to the Conference budget and also exhibited state-of-the-art equipment during the Conference. These were: Gaertner Scientific Co., Rudolph Research Co., and Karl Lambrecht Co.

## LBL RUNAROUND

MMRD didn't dominate the 2nd Annual Runaround like we did the original one when we captured first, second, and third place. However, last year's winner, MMRD's BRIAN TRACY, took second this year. And CATHY COULMAN of the LEVY group was the first woman to cross the finish line. Nice going, BRIAN and CATHY!



NOBEL SYMPOSIUM 47

During the last ten years, the Nobel Foundation has been sponsoring 4 or 5 specialist symposia annually on subjects of great current scientific or cultural interest. The symposia are usually held in some secluded spot near Stockholm, and the attendance is restricted to about thirty invited specialists. Each invitee gives a seminar and there is plenty of discussion, both formal and informal. The final aim is to evaluate the current state of the subject of the symposium and to map out likely future developments.

The 47th symposium in this series was on the "Direct Imaging of Atoms in Molecules and Crystals." It was held on the island of Lidingö, 15 km outside Stockholm. I was fortunate to be one of the participants, despite being the youngest of the 34 scientists invited from Sweden, Norway, Great Britain, France, Germany, Australia, Japan, Canada, and the USA.

There are now three types of instruments capable of directly imaging single atoms: the field ion microscope developed by Muller in Pennsylvania, the scanning transmission electron microscope developed by Crewe in

## NOBEL SYMPOSIUM 47 (Continued)

Chicago, and the fixed beam transmission electron microscope developed by Ruska in Berlin, and recently much improved by the Japanese. The invited seminars covered all three instruments and a range of applications of single atom imaging in physics, biology, materials science, and solid-state chemistry.

Crewe showed his famous color movies of uranium atoms moving on a light substrate, and predicted that in the future it will be possible not only to image single atoms, but also to *individually identify their chemical type* by electron energy loss spectroscopy, a technique in which I have become very interested during the last year. Hashimoto (Osaka) showed very impressive movies of the atomic rearrangements accompanying the motion of twins and stacking faults in crystalline gold. Uyeda (Kyoto) showed beautiful images of biological molecules in which even the light and rather contrastless carbon atoms appeared to be resolved. Horuichi (Ibaraki, Japan) and several others demonstrated how, in structural chemistry, atomic resolution microscopy has now become a routine and powerful structure-solving technique.

Dubochet (Heidelberg) presented a particularly exciting new result: biological molecules cooled to 4°K become 50 to 150 times more resistant to radiation damage than they are at room temperature. This raises much hope for the future of direct atomic imaging in biology, where until now radiation damage (produced by the very electrons used to form the image) has been a major problem.

My own contribution illustrated the power of the direct imaging approach on two long-standing problems from the field of electronic materials. I showed how it is possible to verify the existence of five-fold and seven-fold bonding in an elemental semiconductor by directly imaging high-angle grain boundaries where such bonding

arrangements exist. I also demonstrated how direct imaging reveals the detailed structure of the Si-SiO<sub>2</sub> interface which is the basic working element of MOS (metal-oxide-semiconductor) devices and therefore the most important component in modern electronics.

In all, the symposium powerfully underlined the tremendous development of the direct imaging of atoms during the past decade, and pointed to the enormous range of its practical applications. This is why it's very exciting that the Atomic Resolution Microscope is about to become a reality at Berkeley, thus making LBL a true world leader in this important field.

— O. L. Krivanek

## RESEARCH PROFILE (Continued)

which had not yet been made in macroscopic amounts. My job was to predict the range of possible properties of plutonium metal and provide materials for casting and fabricating the metal, even if it should have the worst possible properties! Such a prediction requires examination of available data for all of the elements and development of models which could be extrapolated. Misleading data made the task especially difficult. For example, the then accepted melting point of uranium was 600° too high.

The worst possible predictions for plutonium indicated that none of the available materials could contain it and that yet undiscovered materials would be needed. Among possible materials, the compound CeS was predicted to have suitable properties. It was prepared for the first time, its predicted properties confirmed, and a factory was set up for the production of crucibles made of CeS and ThS. The crucibles were used at Los Alamos for the casting and fabrication of plutonium metal when it first became available in macroscopic amounts.

## RESEARCH PROFILE (Continued)

### SIGNIFICANCE OF PREDICTIVE MODELS

The philosophy of the approach used in the Manhattan Project has dominated my research. After the war my students carried out experiments to test the models developed earlier. For example, our models could not accommodate the values of the dissociation enthalpy of nitrogen and the enthalpy of sublimation of graphite. When new experimental results in agreement with the predictions of the bonding models were presented, there was great consternation because the previous values were generally accepted by the scientific community. It took more than a decade of repeated checks by a variety of methods before the new values were accepted by the community.

In other instances, such as the study of the vaporization of cuprous chloride, the previous model was found to be deficient. Revised models were developed which predicted that for gases in equilibrium with condensed phases, the complexity of the gaseous species increases with increasing temperature, not only with respect to the number of different species but also to the size of the molecule or degree of polymerization.

Recent attempts to extend the temperature range of new energy processes has provided many examples of unexpected difficulties due to complex gaseous species which become important at very high temperatures.

### TRANSITION METALS

In recent years, research has shifted from high-temperature gases to development of models for predicting the behavior of metallic systems. During the Manhattan Project days, it was demonstrated that CeS could withstand the most electropositive metals; but, surprisingly, platinum attacked it strongly. This indicated the formation of an unusually stable compound of cerium and platinum. In the late forties, Niels Engel, a Danish scientist, spent his sabbatical at Berkeley

writing a manuscript which described a new bonding model for transition metals. He submitted it to several physics journals but the manuscript was rejected because, contrary to the then accepted view that the bonding of Cu, Ag and Au is due to a single s electron per atom with no contribution from d electrons, he insisted that these metals as well as transition metals to the left of the Periodic Table promoted electrons to p orbitals. This provided additional unpaired electrons in the valence state, and enhanced cohesion.

Starting in the mid-sixties, I resurrected Engel's model and found that it was capable of correlating a wide body of data. It was also possible to make fruitful predictions based on his model. I was able to demonstrate that the properties of Cu, Ag and Au could not be reconciled to any bonding model which does not provide for promotion that allows utilization of d electron bonding. Current publications appearing in physics journals almost thirty years after Engel's manuscript was rejected, now begin to acknowledge d-bonding contributions.

An example of the power of the Engel model in obtaining practical results was provided when BOB LAMOREAUX and I were able to tabulate the thermodynamic properties and phase diagrams of 100 binary systems of molybdenum even though no experimental data were available for most systems.

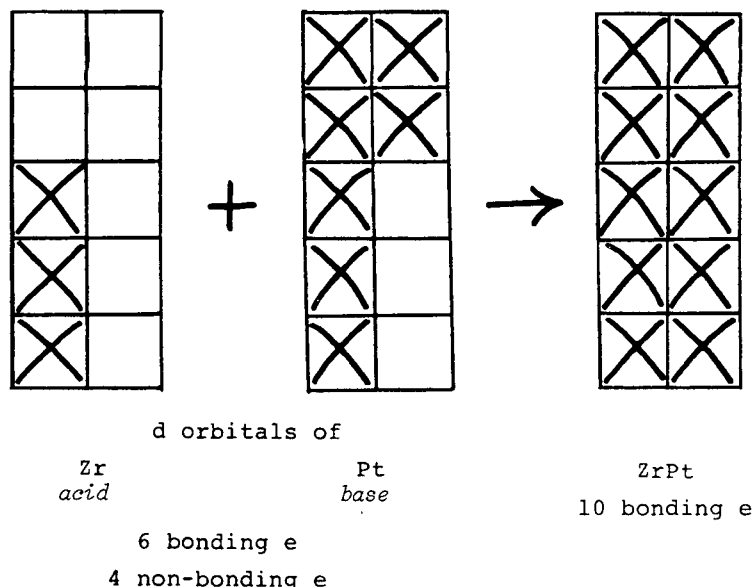
### METALLIC LEWIS-ACID-BASE INTERACTIONS

The Engel theory predicts strong acid-base interactions between platinum group metals and the transition metals of the left side of the Periodic Table with vacant d orbitals, including the lanthanides and actinides. Thus an explanation of the attack of CeS by platinum due to the high stability of CePt<sub>2</sub> is provided. With present models, it is difficult to make accurate predictions for systems with strong acid-base interactions.

The main thrust of our present research is to obtain data that can

# RESEARCH PROFILE (Continued)

## METALLIC LEWIS-ACID-BASE INTERACTIONS



be used to improve the accuracy of existing bonding models. High-temperature solid-electrolyte cells as well as gaseous equilibrium measurements are being used to determine variation of thermodynamic activity with composition in Ta-Ir and Nb-Pd systems. Some of the apparatus used for these studies is also being used to unravel difficulties in the extraction of sulfur dioxide from coal combustion bases and other problems arising in the new high-temperature energy processes.

## THE ENERGY CRISIS

The Department of Energy is trying to set up new energy processes for which most of the data needed to understand the complex high-temperature reactions is lacking. The models that have been developed will play an essential role in predicting chemical behavior and possible new materials to solve problems that arise in this area.

## PEOPLE NEWS

Prof. G. A. SOMORJAI has been invited to present one of the Welch Lectures for 1980. That means at least two of our researchers will be on the Welch schedule — Dr. HEINEMANN and Prof. SOMORJAI.



Dr. SHEREE HSIAO-RU CHEN dedicated her Ph.D. thesis to her parents thusly: "How can the growing grass repay the sun which made it grow?"...

RICHARD J. BUSS, a member of Prof. YUAN LEE's research group, presented an invited report to the American Chemical Society Meeting in Washington, D.C., in September. His presentation, written jointly with LEE, was "Molecular Beam Studies of the Dynamics of Substitution Reactions."



KAREN JANES and her new daughter ERIN visited the Division August 30.

## PEOPLE NEWS (Continued)

JOHN CONWAY is on PRT (Professional Research or Teaching Leave) at the Institute of Nuclear Physics in Orsay, France for several months. He will be working on absorption spectra of actinides in crystals. Expect him back in August, 1980.

Prof. DONALD OLANDER is on sabbatical working at Saclay under the auspices of the French Atomic Energy Agency and living in Paris. He will be studying the basic thermodynamics of fast breeder reactor fuel and visiting many labs and universities around Europe.

DON speaks fluent French, but his sons, ages nine and twelve, do not — yet. Since they will be attending French public schools, however, they will pick it up quickly. The OLANDERS will return in June of next year, but DON expects to be back briefly a couple of times prior to that.

Co-editor, LORETTA LIZAMA, flew off to Hawaii for a too-short vacation just after the August issue of the Newsletter was sent to the printers. She says it was pretty crowded over there, but she managed to get in a lot of activities and came back full of vim, vigor, and poi.

Prof. J. W. MORRIS, Jr. and SUN-KEUN HWANG, now at Rockypoint, New York, but previously a researcher in the Morris group, have obtained U.S. Patent #4,162,158 entitled, "Ferritic Fe-Mn Alloy for Cryogenic Applications."

W. S. YEUNG, previously with the LEVY group at MMRD, has received an appointment as Assistant Professor of Mechanical Engineering at Dartmouth. Congratulations, Prof. YEUNG!

CARL LAMPERT is "acting general editor" of Solar Energy Materials Journal for the next two months while Prof. B. O. Seraphin, the editor, is on vacation in Europe.

MILDRED CHIN has left on maternity leave from her position in the MMRD Personnel Office. We can look forward to her return the first of next year. Our thoughts go with you MILDRED!

SUSAN QUARELLO received her 10-year-service pin as the surprise beginning to a going-away party and baby shower for MILDRED.

DEBBIE JEFFERY, formerly receptionist in the MMRD administration office, has taken a driver-salesman job with Hostess Bakeries. Talk about making a change!

RUTH FLETCHER is the new receptionist in Bldg 62! This is her first experience with a research laboratory as her work in the past has been primarily in private industry.

Away from the job, RUTH likes cooking and sewing — and fishing when she has the opportunity! Welcome, RUTH.

Prof. GARETH THOMAS gave the keynote address at the South East Asia Iron and Steel Institute Congress, Kaohsiung, on September 10th. His topic: "The New World of Duplex Structural Steels."

Taiwan called upon the extensive experience and knowledge of Prof. GARETH THOMAS for assistance in establishing a National Society for Electron Microscopy. He spent the period from September 3 through 19th lecturing extensively at several laboratories and Universities in Taiwan as well as presenting the Keynote Lecture, "Modern Electron Microscopy in Materials Science," at the First R.O.C. Congress, September 11.

Patent #4,152,178 has been assigned to MANOOCH EHR MALEKZADEH and MILTON PICKUS, for a "Sintered Rare-Earth Laves Phase Magnetostrictive Alloy Product and Preparation Thereof."

## PEOPLE NEWS (Continued)

RICHARD LINDBERG has returned to school! RICH, who was in charge of the Electron Microprobe and the Scanning Electron Microscopes, all in Bldg 62, rented a truck and began the long drive east on Sept. 9. He has been accepted for graduate work toward a Master's in Management at Northwestern University. Friends took RICH to lunch and presented him

with a superb briefcase as a going away token.



KENT McARTHUR, WEYLAND WONG, and ROY McCOLLOUGH have been appointed as the MMRD representatives for the annual LBL United Way Campaign which will attempt to better the fine showing of last year.

### LBL REPORTS BY MMRD PERSONNEL

To obtain a copy of any of the LBL/MMRD reports listed below, write directly to the writer whose name is underlined, c/o the Editors, MMRD Newsletter, Bldg. 62, Rm. 209, Lawrence Berkeley Laboratory, Berkeley, CA 94720. If several reports are requested, and the underlined names are different — separate requests are necessary. Nothing more than a postcard is needed, and if several are ordered at one time, use 3 x 5 cards in one envelope.

LBL-6044: Molecular Beam Study of the Kinetics of the Fluorine-Uranium Dioxide Reaction .... A. J. Macbiels and D. R. Olander

LBL-6278 Rev. II: Precipitation-Strengthened Austenitic Fe-Mn-Ti Alloys .... K. M. Chang and J. W. Morris, Jr.

LBL-6993 Rev.: High Temperature Stress-Strain Behavior of MgO in Compression .... P. C. Dokko and J. A. Pask

LBL-7399: Radiation Damage Studies by X-Ray Photoelectron Spectroscopy: III. Electron Irradiated Halates and Perhalates .... T. Sasaki, R. S. Williams, J. S. Wong, and D. A. Shirley

LBL-8069: Diffusion of a Chemical Species Through a Viscous Boundary Layer .... J. Keller (A. Levy)

LBL-8310: Structure and Mechanical Properties of Fe-Cr-Mo-C Alloys With and Without Boron .... G. Thomas and Y.-L. Chen

LBL-8442: Transformation Toughening in Ceramics: Martensitic Transformations in Crack Tip Stress Fields .... A. G. Evans and A. H. Heuer

LBL-8448: Coherent Brillouin Spectroscopy .... A. G. Jacobson and Y. R. Shen

LBL-8461: Microstructure and Ionic Resistivity of Calcium Containing Sodium Beta Alumina .... A. Buechele and L. C. De Jonghe

LBL-8472: Structure Sensitivity in the Electrocatalytic Properties of Pt: I. Hydrogen Adsorption on Low Index Single Crystals and the Role of Steps .... P. N. Ross, Jr.

LBL-8496: Wetting and Adherence of Na-Borate Glass on Gold .... S. T. Tso and J. A. Pask

LBL-8504: Ge:Ga Photoconductors in Low Infrared Backgrounds .... E. E. Haller, M. R. Hueschen, and P. L. Richards

LBL-8628: Design of Duplex Low-Carbon Steels with Carbide Forming Elements .... P. K. Costello (M.S. Thesis) (G. Thomas)

LBL-8632 Rev.: Microstructure and Optical Properties of Black Chrome Before and After Exposure to High Temperatures .... C. M. Lampert and J. Washburn

LBL-8638: Josephson Effect Devices .... J. Clarke

LBL-8652: Vibrational Dephasing of Polyatomic Molecules in Condensed Phases. II. Temperature Dependence of Raman Spectral Lines Resulting from Energy

- Exchange in 1,2,4,5-Tetramethylbenzene .... P. A. Cornelius, R. M. Shelby and C. B. Harris
- LBL-8681: Soft X-Ray Absorption Spectroscopy: Electronic and Morphological Structure of Polyvinylidene Fluoride .... R. S. Williams, D. Denley, D. A. Shirley, and J. Stöhr
- LBL-8684: Gas/Solid Reactions: Hydrogen Reduction of Cobalt Ferrites and  $Al^{3+}$  Containing Cobalt Ferrites .... M. C. Rey and L. C. De Jonghe
- LBL-8692: High Temperature Failure Mechanisms in Ceramics .... A. G. Evans and A. Rana
- LBL-8929 Abst.: Enhancement of Chemical Reactions by Collision Induced of Infrared Laser Radiation .... A. E. Orel and W. H. Miller
- LBL-8996: Surface Structures of Metallic Monolayers on Metal Crystal Surfaces .... J. P. Biberian and G. A. Somorjai
- LBL-9021: Electron Spectroscopy Studies of Clean Oxide Surfaces, Chemisorbed Molecules and Photo-Assisted Processes .... W. J. Lo (Ph.D. Thesis) (G. Somorjai)
- LBL-9103: The Effects of Air Melting on Fe/0.3C/3Cr/0.5Mo/2Mn and Fe/0.3C/3Cr/0.5Mo/2Ni Structural Alloy Steels B. Steinberg (M.S. Thesis) (G. Thomas)
- LBL-9170: Selective Resonant Enhancement of Electron Correlation Satellites in Atomic Barium .... R. A. Rosenberg, M. G. White, G. Thornton, and D. A. Shirley
- LBL-9197: On the Quantum Mechanical Implications of Classical Ergodicity .... R. M. Stratt, N. C. Handy, and W. H. Miller
- LBL-9207: Studies on the Electrochemical Behavior of Potassium in Propylene Carbonate .... H. H. Law (Ph.D. Thesis) (C. Tobias and R. Muller)
- LBL-9219: Photodissociation Processes in Molecular Beams .... L. R. Carlson (Ph.D. Thesis) (Y. T. Lee)
- LBL-9257: Microstructure, Sintering and Strength of Polycrystalline SiC .... M.-F. Sung (M.S. Thesis) (G. Thomas)
- LBL-9260: Alloying and Heat Treatment Optimization of Fe/Cr/C Steels for Improved Mechanical Properties .... M. Sarikaya (M.S. Thesis) (G. Thomas)
- LBL-9262: The Effect of Air-Cooling Heat Heat Treatments on the Structure and Properties of Fe/4Cr/0.3C/2Mn Alloy .... T. H. Rabe (M.S. Thesis) (G. Thomas)
- LBL-9264: The Computer Simulation of Martensitic Transformations in Idealized Systems .... S. H.-R. Chen (Ph.D. Thesis) (J.W.Morris, Jr.)
- LBL-9265: Ellipsometry of Sulfate Films on Lead .... R. H. Muller and R. D. Peters
- LBL-9266: DC Squid: Current Noise .... C. D. Tesche and J. Clarke
- LBL-9280: The Chemisorption of CO and  $CO_2$  on Rh(111) Studied by High Resolution Electron Energy Loss Spectroscopy .... L. H. Dubois and G. A. Somorjai
- LBL-9288: LEED, AES and Thermal Desorption Studies of the Oxidation of the Rhodium (111) Surface .... D. G. Castner and G. A. Somorjai
- LBL-9308: The Effect of Coal Char on the Corrosion of 304 SS .... T.F.W.Foerster (M.S. Thesis) (J. Newman)
- LBL-9319: Iodine Stress-Corrosion Cracking of Zircaloy .... S.-H. Shann and D. R. Olander
- LBL-9324: Metal Foils for Direct Application of Absorber Coatings on Solar Collectors .... C. M. Lampert (J. Washburn)
- LBL-9341: Surface Coherent Anti-Stokes Raman Spectroscopy .... C. K. Chen, A. Rubens, B. de Castro, Y. R. Shen, and F. DeMartini
- LBL-9346: Computer Simulation of the Martensite Transformation in a Model Two-Dimensional Body .... S. Chen, A. G. Khachaturyan, and J. W. Morris, Jr.

- LBL-9351: Improved *Ab Initio* Effective Core Potentials for Molecular Calculations .... P. A. Christiansen, Y. S. Lee, and K. S. Pitzer
- LBL-9358 Abst.: Energetics and Dynamics of Molecule-Ions by Photoionization of Van der Waals Molecules .... S. Ceyer, P. Tiedemann, T. Hirooka, S. Anderson, B. H. Mahan, and Y. T. Lee
- LBL-9363: A New Microfacet Notation for High-Miller-Index Surfaces of Cubic Materials with Terrace, Step and Kink Structures .... M. A. Van Hove and G. A. Somorjai
- LBL-9374: Direct Measurements of the Spectrum of the Near-Millimeter Cosmic Background .... P. L. Richards
- LBL-9384: Condensed Phase Photoelectron Asymmetry .... R. F. Davis, S. D. Kevan, B.-C. Lu, J. G. Tobin, and D. A. Shirley
- LBL-9396: Geochemical and Cosmochemical Cycles Involving Sulfur, Sulfide, Sulfite, and Sulfate .... B. Meyer, L. Peter, and M. Ospina (L. Brewer)
- LBL-9398: Measurement of Refractive Indices and Study of Isotropic-Nematic Phase Transition by the Surface Plasmon Technique .... K. C. Chu, C. K. Chen, and Y. R. Shen
- LBL-9404: Periodic Phenomena During Anodic Dissolution of Copper at High Current Densities .... J. F. Cooper, R. H. Muller, and C. W. Tobias
- LBL-9422: Core Level Satellite Structure in Photoemission Spectra of Transition Metals .... J. Tersoff, L. M. Falicov, and D. R. Penn
- LBL-9430: Angle-Resolved Photoemission Determination of  $\Lambda$ -Line Valence Bands in Pt and Au Using Synchrotron Radiation .... K. A. Mills, R. F. Davis, S. D. Kevan, G. Thornton, and D. A. Shirley
- LBL-9431: Carbon K-Edge Fine Structure in Graphite Foils and in Thin-Film Contaminants on Metal Surfaces .... D. Denley, P. Perfetti, R. S. Williams, D. A. Shirley, and J. Stöhr
- LBL-9457: On the Law of Mixtures in Dual-Phase Steels .... J. Y. Koo, M. J. Young, and G. Thomas
- LBL-9478: Structure of Tris(urea)dioxo-uranium(VI) Sulfate,  $\text{UO}_2(\text{OC}(\text{NH}_2)_2)_3\text{SO}_4$  .... H. Ruben, B. Spencer, D. H. Templeton, and A. Zalkin
- LBL-9488: The Kinetics of Reaction of Porous CaO Powders with Water Vapor .... D. Beruto and A. W. Searcy
- LBL-9514: Coordination Chemistry of Metal Surfaces — Carbon Monoxide Chemisorption States on Pt(111) .... C. M. Friend, R. M. Gavin, E. L. Muetterties, and M.-C. Tsai
- LBL-9518: Supercurrent-Induced Charge Imbalance Measured in a Superconductor in the Presence of a Thermal Gradient .... J. Clarke, B. R. Rjordbøge and P. E. Lindelof
- LBL-9528: Enhancement of the Energy Gap in Superconducting Aluminum by Tunneling Extraction of Quasiparticles .... C. C. Chi and J. Clarke
- LBL-9529: Fatigue in Ceramics .... A. G. Evans
- LBL-9530: Polarized X-Ray Absorption and Double Refraction in Vanadyl Bisacetyl-acetate .... D. H. Templeton and L. K. Templeton
- LBL-9555: Ozone Photolysis: A Determination of the Electronic and Vibrational State Distributions of Primary Products R. K. Sparks, L. R. Carlson, K. Shobatake, M. L. Kowalczyk, and Y. T. Lee
- LBL-9559: Theory of Quasiparticle Charge Imbalance Induced in a Superconductor by a Supercurrent in the Presence of a Thermal Gradient .... J. Clarke and M. Tinkham
- LBL-9561: Branch Imbalance Relaxation Times in Superconductors .... J. Clarke, U. Eckern, A. Schmid, G. Schön and M. Tinkham

LBL-9571: A New Equation of State for Fluid Water Based on Hard-Sphere Perturbation Theory and Dimerization Equilibria .... W. B. Whiting and J. M. Prausnitz

LBL-9575: Hydrogen-Deuterium Exchange; Perdeutero-Hydridotris(hexamethyl-disilyl)amido-Thorium(IV) and -Uranium (IV) .... S. J. Simpson, H. W. Turner, and R. A. Andersen (N. Edelstein)

LBL-9577: Boundary Resistance of the Superconducting-Normal Interface .... T. Y. Hsiang and J. Clarke

LBL-9596: Surface and Adsorbate Structural Studies by Photoemission in the  $h\nu = 50\text{-}500$  eV Range .... D. A. Shirley

LBL-9607: Instantaneous Global Ozone Balance Including Observed Nitrogen Dioxide .... S. Solomon, H. S. Johnston, M. Kowalczyk, and I. Wilson

LBL-9637: Semiclassical Statistical Mechanics of Fluids. II. An Improved Mean Field Effective Pair Potential .... R. M. Stratt (W. H. Miller)

LBL-9687 Abst.: Molecular Beam Studies of the Dynamics of Substitution Reactions .... R. J. Buss and Y. T. Lee

LBL-9688 Abst.: Reaction Dynamics of  $F + H_2, D_2$  .... R. K. Sparks, C. C. Hayden, K. Shobatake, and Y. T. Lee

## CALENDAR

October 1979: International Energy Conservation Month

October 4-5: 7th Summer Roundtable on "Liquid Chromatography," Holiday Inn, Emeryville, and USDA, Albany.

October 10-12: Conference on "Chemistry and Spectroscopy," Huntington-Sheraton Hotel, Pasadena, CA. Subjects: Mini-computers, ion selective electrodes, gas chromatography/mass spectrometry equipment, employment and research opportunities.

**SURFACE SCIENCE AND CATALYSIS SEMINARS, 4:00 p.m., Bldg 62, Rm 203:**

October 3: "Surface Penning Ionization: Theory and Application as a New Technique for the Analysis Chemisorbed Systems," by S. W. Wang, Stanford University.

## SURFACE SCIENCE AND CATALYSIS (Con't)

October 10: "Photocatalytic Dissociation of Water," by G. A. Somorjai, Univ. of California.

October 17: "Catalytic and Surface Properties of Activated Lanthanum Sesquioxide," by M. P. Rosynek, Texas A&M University.

October 24: "Acid Catalyzed Reactions on Zeolites," by W. O. Haag, Mobil Research & Development Corp.

October 31: "Hot Carrier Effects at Illuminated Semi-Conductor Electrolyte Interfaces," by A. J. Nozik, SERI.

November 1979: AiChE Annual Meeting, San Francisco, C. J. King, Program Chairman.

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SECOND CLASS MAIL

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