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Capt Lee E. Myers

22b. TELEPHONE NUMBER
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(202) 767-4963

22c. OFFICE SYMBOL

NC

First International Conference on the Structure of Surfaces (ICSOS-1)
Berkeley, California
August 13-16, 1984

AFOSR-TR-89-177

Schedule of Presentations

All oral sessions will be held in the Sibley Auditorium of the Bechtel Engineering Center of the University of California campus.

All poster sessions and coffee breaks will be held in Room 120, one floor below Sibley Auditorium.

INV indicates invited presentations.

Monday, August 13, 1984 (Deadline for Manuscript Submission)

- 8:00-17:30 Registration in lobby by Sibley Auditorium (Also 8:00-17:30 August 14-16)
- 8:30-18:00 First half of commercial exhibit—Room 120
- 8:30 INTRODUCTION—S.Y. Tong
- 8:40-10:20 A. *STRUCTURAL TECHNIQUES I*—S.Y. Tong, Presiding
- 8:40 A1 INV F. Jona
Determination of Surface Structure by LEED
- 9:20 A2 INV M. Aono, R. Souda, C. Oshima and Y. Ishizawa
Structure Analysis of Semiconductor and Inorganic Compound Surfaces
by Impact Collision Ion Scattering Spectroscopy
- 10:00 A3 INV J. Tersoff
Theory of the Scanning Tunneling Microscope
- 10:20-10:50 COFFEE BREAK—Room 120
- 10:50-12:10 B. *CLEAN METALS*—J.R. Smith, Presiding
- 10:50 B1 INV M. Rocca, H. Ibach, S. Lehwald, B.M. Hall, M.L. Xu and S.Y. Tong
Electron-Phonon Scattering and Structure Analysis
- 11:10 B2 INV J.C. Lapujoulade, B. Salanon and D. Gorse
Surface Structure Analysis by Atomic Beam Diffraction
- 11:50 B3 INV J.R. Noonan and H.L. Davis
Several Faces of Aluminum
- 12:10-14:00 LUNCH BREAK
- 14:00-16:00 C. *MOLECULAR ADSORPTION I*—A.M. Bradshaw, Presiding
- 14:00 C1 INV T.H. Upton
Determining Molecular Adsorbate Structures from Adsorbate Electronic Properties
- 14:40 C2 INV M.A. Van Hove
Structure Determination of Molecular Adsorbates with Dynamical LEED and HREELS
- 15:20 C3 INV J. Stöhr
SEXAFS and NEXAFS Studies of Chemisorbed Molecules: Bonding and Structure
- 16:00-18:00 D. *TECHNIQUES, ORDERING*—posters (and refreshments)—Room 120
- D1 P.H. Fuoss and A. Fischer-Colbrie
Structural Studies of Ultra-Thin Amorphous Layers on Surfaces
- D2 K.S. Liang, P.H. Fuoss, G.J. Hughes and P. Eisenberger
Synchrotron X-Ray Scattering Study of Chemisorption System: Oxygen on Cu(110) Surface
- D3 K.H. Lee, M.H. Lee and H.I. Zhang
Boundary and Size Effects on Frequencies of a Finite Simple Cubic
Lattice with Coherently Adsorbed Surface Layers

Chemical Information Division

23 SEP 85

AFSC

- D4 R.H. Howell, P. Meyer, I.J. Rosenberg and M.J. Fluss
A New Capability for the Study of Surfaces with Intense Positron Beams
- D5 H.G. LeDuc, A.P. Thakoor, J. Lambe and S.K. Khanna
Influence of Adsorbates on Surface States of (111) Gold Observed
by Electron Tunneling and Electoreflectance
- D6 A.N. Jette, C.B. Barger and B.H. Nall
Dynamical Computations of Current Image Diffraction Images (CID)
- D7 T. Hsu and J.M. Cowley
REM Studies of Crystal Lattice Terminations at Surfaces
- D8 S. Ferrer and C. Ocal
Electronic Properties of Small Gold Deposits on Very Thin Aluminum Oxide
Layers. The Appearance of Subsurface Gold
- D9 C.R. Aita, C.J. Kubiak, N.C. Tran and T.L. Barr
X-Ray Photoelectron Loss Spectroscopy of Wide Energy Band Gap Aluminum Compounds
- D10 I. Bartoš and J. Koukal
On the Role of Space Inhomogeneity of Electron Damping in LEED
- D11 R. Mayol, F. Salvat and J. Parellada-Sabata
Attenuation of Isotropically Emitted Electron Beams
- D12 K. Müller and K. Heinz
Computer Controlled LEED Intensity and Spot Profile Determination
- D13 N.C. Bartelt, T.L. Einstein and L.D. Roelofs
Structure Factors for Adsorbed Overlayers from Monte Carlo and
Convenient Methods for Analysis of LEED Data Near Phase Transitions
- D14 J.M. Pimbley, P. Fenter and T.-M. Lu
Short Range Correlations in Imperfect Surfaces and Overlayers
- D15 D. Saloner and M.G. Lagally
Domain-Size Determination in Heteroepitaxial Systems from LEED Angular Profiles
- D16 D.D. Vvedensky, D.K. Saldin and J.B. Pendry
Near-Edge X-Ray Absorption Spectroscopy
- D17 D.K. Saldin, D.D. Vvedensky and J.B. Pendry
The Structure of Organic Adsorbates from Elastic Diffuse LEED
- D18 M. Drechsler
The Structure of Faces and Steps on Hexagonal Metals
- D19 E.A. Conrad, D.S. Kaufman, R. Aten and T. Engel
Quantitative Studies of Stepped Ni and Cu Surfaces Using Helium Diffraction
- D20 P.R. Pukite, C.S. Lent and P.I. Cohen
Diffraction From A Disordered Staircase
- D21 F.F. Abraham
Computer Simulations of Surfaces, Interfaces and Physisorbed Films
- D22 J.C. Campuzano, M.S. Foster, R.F. Willis and W. Unertl
Determination of the Critical Exponents of the $\text{Au}(110)(1 \times 2) \leftrightarrow (1 \times 1)$
Phase Transition
- D23 S.C. Ying and G.Y. Hu
Theory of Commensurate-Incommensurate Phase Transitions on H/W(001)
- D24 R.J. Behm, K. Christmann, G. Ertl, V. Penka and R. Schwankner
Competing Reconstruction Mechanisms in H/Ni(110)
- D25 T. Aruga, H. Tochiyama and Y. Murata
Low-Energy Electron Diffraction Studies of K Monolayers on Cu(001)
- D26 K.M. Martini, S. Burdick, M. El-Batanouny and G. Kirczenow
Molecular Dynamics Investigation of Dislocation-Depinning Transitions
in Mismatched Overlayers
- D27 S.M. Levine and S.H. Garofalini
Molecular Dynamics Simulations of Pt Adatoms on the Vitreous Silica Surface



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Tuesday, August 14, 1984

8:30–18:00 Continuation of first half of exhibit.

8:30–10:10 *E. DISORDER, DEFECTS*—M.B. Webb, Presiding

8:30 E1 INV J.B. Pendry and D.K. Saldin

LEED, XANES and the Structure of Disordered Surfaces

9:10 E2 M. Ringger, H.R. Hidber, R. Schlögl, P. Oelhafen, H.-J. Güntherodt,
K. Wandelt and G. Ertl

The Surface Topography of a Pd Single Crystal Studied by the
Scanning Tunneling Microscope

9:30 E3 INV M. Henzler

Quantitative Analysis of Spot Profiles of LEED

10:10–10:40 COFFEE BREAK—Room 120

10:40–12:00 *F. STRUCTURAL TECHNIQUES II*—W.E. Spicer, Presiding

10:40 F1 INV C.J. Wright

Surface Characterization by the Inelastic Scattering of Neutrons from Adsorbates

11:20 F2 INV C.P. Slichter

NMR and Surface Structure

11:40 F3 W.F. Egelhoff, Jr.

X-Ray Photoelectron and Auger Electron Forward Scattering: A New
Tool for Studying Epitaxial Growth and Core-Level Binding-Energy Shifts

12:00–14:00 LUNCH BREAK

14:00–16:00 *G. MOLECULAR ADSORPTION II*—G.A. Somorjai, Presiding

14:00 G1 INV T.E. Madey

The Uses and Limitations of ESDIAD for Determining the Structure of Surface Molecules

14:40 G2 A. Puschmann, K.C. Prince, J. Haase, G. Paolucci and A.M. Bradshaw

Photoemission and SEXAFS Studies of Oxygen Overlayers on Ag(110)

15:00 G3 INV N.V. Richardson

The Characterization of Adsorbed Molecules by Electron Energy Loss Spectroscopy

15:40 G4 INV Y.R. Shen

Optical Second-Harmonic Generation for Surface Studies

16:00–18:00 *H. SEMICONDUCTORS, INSULATORS*—posters (and refreshments)—Room 120

H1 I.P. Batra, F.J. Himpsel, P. Marcus, R. Tromp, M.R. Cook, F. Jona, and H. Liu
Structure of Si(111) Surfaces

H2 R.M. Tromp, L. Smit and J.F. van der Veen
Ion Beam Analysis of the Si(111)-(2×1) Surface

H3 R.M. Tromp and E.J. van Loenen
Evaluation of Si(111)-(7×7) Structure Models by Channeling and Blocking

H4 C.D. Chen, A. Selloni and E. Tosatti
Structure and Temperature Dependent Polaron Shifts on Si(111) 2×1

H5 Y.S. Shu, W.S. Yang, F. Jona and P.M. Marcus
Refinement of the Buckled Dimer Model for Si{001}2×1

H6 B.W. Holland, C.B. Duke and A. Paton
The Atomic Geometry of Si(100)-(2×1): Resolution of Incompatibility
between ELEED and Ion Scattering

H7 D.C. Allan and E.J. Mele
Surface Vibrational Excitations for Si(100)2×1

H8 A. Sakai, M.J. Cardillo, W.R. Lambert, P. Trevor and J. Tersoff
The Structures of the Ge(100) and Si(100) Surfaces as Probed by He Diffraction

- H9 H.H. Farrell, J.Q. Broughton, F. Stucki and J.C. Bean
Shape Resonances in OH/Semiconductor Systems
- H10 A. Taleb-Ibrahimi, C. Sébenne and F. Proix
Metal Induced Reconstructions on Cleaved Silicon (111) at Room Temperature
- H11 G. Le Lay and J.P. Bibérian
Metal-Induced Reconstructions of Silicon, Germanium and Diamond
Low-Index Surfaces
- H12 S.B. Zhang, J.E. Northrup and M.L. Cohen
Theory of the Structure of the Ge-Si(111) Interface
- H13 J.A. Yarmoff and R.S. Williams
Low-Energy Ion-Backscattering Angular Distributions from Clean and
Absorbate-Covered Ge Surfaces
- H14 M.A. Olmstead and N.M. Amer
Polarization Dependent Ge and Si(111) Surface State Optical Absorption:
A Probe of Surface Structure
- H15 J.E. Northrup
The Arsenic Terminated Ge(111) Surface
- H16 Y.N. Xu, K.M. Zhang and X.D. Xie
Studies on the Fermi Level Pinning of GaAs(110) Surfaces
- H17 F. Bartels and W. Möñch
Chemisorption of Oxygen at Cleaved GaAs(110) Surfaces: Work Function
and Surface Band-Bending
- H18 O. Nishikawa, O. Kaneda, M. Shibata and E. Nomura
Atom-Probe Study of Al-Ga Exchange Reaction on GaAs Surfaces
- H19 G. Xu, W.N. Mei and S.Y. Tong
A Vacancy-Buckling Model for the (2×2) GaAs(111) Surface
- H20 R.D. Bringans and R.Z. Bachrach
A Comparison between the Electronic Properties of GaAs(111) and GaAs($\overline{111}$)
- H21 P. Hren, D.W. Tu and A. Kahn
Atomic Structure of GaAs(211)
- H22 C.B. Duke, C. Mailhot, A. Paton, K. Li, C. Bonapace and A. Kahn
Atomic Geometries of (1×1) Sb Overlayers on GaAs(110) and InP(110)
- H23 R.L. Johnson, J.H. Fock, J. Bohr, R. Feidenhansl, J. Als-Nielsen,
M. Nielsen and M. Toney
Surface X-Ray Diffraction from the Polar (111) Surfaces of InSb
- H24 L. Smit, T.E. Derry and J.F. van der Veen
Atomic Structure of Clean and Al Covered III-V Compound Cleavage Faces
- H25 J.M. Nicol, J. Howard and J. Eckert
IR and Neutron Spectroscopy of Hydrogen and Ethylene Adsorbed on Type A Zeolites
- H26 J. Eckert, B.H. Grier, L. Passell, H. Patterson, D. Richter and R. Rollefson
Structures and Dynamics of Ethylene Surface Layers on Graphite
- H27 N.J. Wu and A. Ignatiev
C(0001)-(2×2)K Surface Intercalated Structure

18:30 Dinner meeting for International Organizing Committee. Faculty Club, Berkeley Campus

Wednesday, August 15, 1984

8:30-18:00 Second half of commercial exhibit—Room 120

8:30-10:10 I. *ATOMIC ADSORPTION*—L.M. Falicov, Presiding

8:30 I1 INV J.K. Nørskov and S. Holloway

The Binding of Adsorbates to Metal Surfaces

9:10 I2 R.W. Godby, R. Haydock and V. Heine

Bonding and Interaction of Oxygen Atoms on Nickel (001) from Self-Consistent Electronic Structure

9:30 I3 INV J.J. Barton, S.W. Robey, C.C. Bahr and D.A. Shirley

Surface Structure Determination with ARPEFS

9:50 I4 INV E.L. Bullock, C.S. Fadley, B.L. Hermsmeier, M. Sagurton,

R. Saiki, B. Sinkovic and R. Trehan

Photoelectron Diffraction and Surface Structures: Future Prospects

10:10-10:40 COFFEE BREAK—Room 120

10:40-12:00 J. *SEMICONDUCTORS I*—X.D. Xie, Presiding

10:40 J1 INV Y.J. Chabal

High-Resolution Infrared Spectroscopy and Surface Structure

11:20 J2 INV Y. Petroff

Low-Temperature Photoemission on Semiconductors

11:40 J3 INV D. Vanderbilt and S.G. Louie

Energy Minimization Calculations for Diamond (111) Surface Reconstructions

12:00-14:00 LUNCH BREAK

14:00-16:00 K. *ADSORBATE-ADSORBATE INTERACTIONS*—R.J. Madix, Presiding

14:00 K1 INV R.J. Birgeneau

Phases and Phase Transitions in Systems with Competing Interactions

14:40 K2 J. Ochab, W.N. Unertl, P.H. Kleban, G. Akinici, P. Bak,

N.C. Bartelt and T.L. Einstein

The Ashkin-Teller Model and the Ordered Phases of Se/Ni(100)

15:00 K3 INV G. Ehrlich

Surface Diffusion and Adatom-Adatom Interactions

15:40 K4 INV T.T. Tsong

An Atom-Probe and Field Ion Microscope Study of the Atomic Structure and Composition of Metal Surfaces

16:00-16:30 INFORMAL RECEPTION—Room 120

16:00-18:00 L. *METALS AND ADSORBATES*—posters—Room 120

L1 R. Richter, J.R. Smith and J.G. Gay

Total Energies and Atom Locations at Solid Surfaces

L2 K.M. Ho and K.P. Bohnen

Investigations of Multilayer Relaxation on Metal Surfaces Using Self-Consistent Electronic Structure Calculations

L3 H.L. Davis and G.-C. Wang

Layer Relaxation of the Clean W(112) Surface and Its Variation with Adsorbed Oxygen

L4 Y. Gauthier, Y. Joly, R. Baudoing and J. Rundgren

Oscillatory Behavior of Some Surface Properties—Interlayer Distances in Metals and Composition in Binary Alloys

L5 H.-J. Brocksch and K.H. Bennemann

Theoretical Study of the Structural Stability of the Reconstructed (110)-Surfaces of Ir, Pt, and Au

- L6 T. Takai, T. Halicioğlu and W.A. Tiller
The Structure and Surface Energy of Au(110): Studied by Monte Carlo Method
- L7 C.-M. Chan and M.A. Van Hove
A Comparison of the Missing-Row Model and Several Proposed Models for the Reconstructed Ir(110)-(1×2) Surface
- L8 U. Bardi, M. Torrini, E. Zanazzi, G. Rovida, M. Maglietta, P.N. Ross and M.A. Van Hove
Structure of the Pt₃Ti(001) Surface by LEED Dynamical Intensity Analysis
- L9 A.D. Tenner, K.T. Gillen, T.C.M. Horn, J. Los and A.W. Kleyn
Surface Rainbow Scattering of Alkali Ions from W(110)
- L10 S.H. Overbury, D.R. Huntley and W.E. Brower, Jr.
Structural Studies of the Surface of Amorphous Fe₈₀B₂₀ by Low Energy Alkali Ion Scattering
- L11 S.H. Overbury, B.M. DeKoven and P.C. Stair
Low Energy Alkali Ion Scattering as a Probe of Adsorbate Ordering
- L12 C. Umrigar and J.W. Wilkins
Determination of the Geometry of Adsorbates on Surfaces Via Total Energy Calculations: H/Ni(100)
- L13 M.S. Daw and S.M. Foiles
Application of the Embedded Atom Method to H on Ni and Pd Surfaces
- L14 M. Sagurton, E.L. Bullock and C.S. Fadley
Single-Scattering Analysis of Off-Normal Photoelectron Diffraction Data
- L15 W.N. Mei, H.C. Poon and S.Y. Tong
Fourier Transformation of Dynamical and Kinematical Energy Dependent Photoelectron Diffraction (EDPD) Spectra—A Theoretical Analysis
- L16 I.P. Batra, T. Engel and K.H. Rieder
Helium Diffraction from Oxygen Covered Nickel Surfaces
- L17 P.S. Bagus, C.W. Bauschlicher, Jr. and C.J. Nelin
Scattering of He from O/Ni(100): Cluster Model Studies
- L18 C.W. Bauschlicher, Jr., P.S. Bagus and K.E. Hermann
The Bonding of Closed Shell Molecules to Transition Metal Surfaces
- L19 D. Tománek and K.H. Bennemann
Total Energy Calculations for the Adsorption of N₂ and NO on Fe(111)
- L20 M.A. Passler
Surface Structure of NO Adsorbed on Ni(011)
- L21 C.M. Mate and G.A. Somorjai
Surface Structure of Fluorobenzene, Chlorobenzene, and Pyridine Adsorbed on Rh(111) Studied by HREELS
- L22 D.F. Ogletree, M.A. Van Hove and G.A. Somorjai
Low-Energy Electron Diffraction Study of the Structure of Benzene Adsorbed on Pt(111)
- L23 J.L. Stickney, S.D. Rósasco, G.N. Salaita and A.T. Hubbard
Ordered Ionic Layers Formed on Pt(111) from Aqueous Solutions
- L24 A.P. Alivisatos, D.H. Waldeck and C.B. Harris
The Electronic Structure of Metals and Their Ability to Quench Molecular Excited States
- L25 G.M. Goncher, C.A. Parsons and C.B. Harris
Surface Resonance Enhanced Multiphoton Fragmentation on Rough Metal Surfaces

Thursday, August 16, 1984

8:30-17:30 Continuation of second half of exhibit—Room 120

8:30-10:10 *M. SEMICONDUCTORS II*—D.R. Hamann, Presiding

8:30 M1 INV M.L. Cohen
Theory of Surface Reconstruction

9:10 M2 INV E.G. McRae
Triangle-Dimer Stacking-Fault Model of the Si(111)-(7×7) Surface
Bonding Configuration

9:50 M3 INV P. Chiaradia
Optical Transitions and Surface Structure

10:10-10:40 COFFEE BREAK—Room 120

10:40-12:00 *N. ORDERING*—J.B. Pendry, Presiding

10:40 N1 INV S.C. Fain, Jr. and H. You
LEED Studies of Structures and Phase Transitions of Physically
Adsorbed Nitrogen and Carbon Monoxide Molecules on Graphite

11:20 N2 INV M.B. Webb
LEED Studies of Physisorbed Noble Gases on Metals and the Interatom Interactions

11:40 N3 S. Brennan, P.H. Fuoss and P. Eisenberger
X-Ray Scattering Studies of the Structure and Melting of Pb on Cu (110) Surfaces

14:00-15:40 *O. INTERFACES*—R.Z. Bachrach, Presiding

14:00 O1 INV L.M. Falicov and R. Victora
Magnetic Properties of Transition Metal Surfaces and Overlayers

14:20 O2 INV P.H. Citrin
Current Status and Future Directions of Surface-EXAFS

15:00 O3 INV F.A. Ponce
Direct Observation of the Structure of Interfaces Using Atomic-Resolution
Electron Microscopy

15:40-16:10 REFRESHMENTS—Room 120

16:10-17:30 *P. METAL RECONSTRUCTION*—D.J. Chadi, Presiding

16:10 P1 INV I.K. Robinson
Surface Structure by X-Ray Diffraction

16:50 P2 INV R.F. Willis
W(100) Surface Structural Phase Transformations: Current Models, Theory and Experiment

17:30 END OF ICSOS-I

JAN 22 1985

Abstract of Proceedings

These Proceedings are a collection of selected papers presented at the First International Conference on the Structure of Surfaces (ICSOS-1). They assess the status of surface structural determination and the relationship between surface or interface structures and physical or chemical properties of interest. This includes solid and adsorbate-covered surfaces, well-established and promising new surface-sensitive techniques, experiment and theory.

FIRST INTERNATIONAL CONFERENCE
ON THE STRUCTURE OF SURFACES (ICSOS)

R O S T E R

Lawrence Berkeley Laboratory
Berkeley, California

Carolyn R. Aita
University of Wisconsin
Lab for Surface Studies & Material
P. O. Box 784
Milwaukee, WI 53201

(414) 963-4733

Douglas C. Allan
University of Pennsylvania
Department of Physics
Philadelphia, PA 19104

(215) 898-5987

Lynn R. Allen
University of Washington
BG-10, Department of Chemistry
Seattle, WA 98195

(206) 545-2594

N. M. Amer
Lawrence Berkeley Laboratory
Bldg. 70, Room 110A
Berkeley, CA 94720

(415) 486-5601

Masakazu Aono
National Institute for Research
in Inorganic Materials
1-1 Namiki, Sakura-Mura
Niihara-Gun, Ibaraki, 305, JAPAN

(0290) 51 3351, ext. 251

Walter E. Atkinson
Riverside Research Institute
1701 North Fort Myer Drive
Arlington, VA 22180

(703) 522-2310

Robert Z. Bachrach
Xerox, P.A.R.C.
3333 Coyote Hill Road
Palo Alto, CA 94304

(415) 494-4157

Paul S. Bagus
IBM Research Laboratory
K33/281, 5600 Cottle Road
San Jose, CA 95193

(408) 256-7663

John J. Barton
Bldg. 70A, Rm. 1115
Lawrence Berkeley Laboratory
Berkeley, CA 94720

(415) 486-5666

Igor Bartos
University of Waterloo
Department of Applied Mathematics
Waterloo, Ontario N2L 3G1
CANADA

(519) 885-1211 ext 3471

Inder P. Batra
IBM Corporation K33/281
5600 Cottle Road
San Jose, CA 95193

(408) 256-7325

Bauschlicher
NASA AMES
STC-230-3
Moffett Field, CA

(415) 965-6231

R. Juergen Behm
University of Munchen, F.R.G.
Sophiensn. 11
D-8000 Munchen 2
WEST GERMANY

Peter A. Bennett
Arizona State University
Physics Department
Tempe, AZ 85287

(602) 965-5218

Brian E. Bent
MMRD, Building 62
Lawrence Berkeley Laboratory
Berkeley, CA 94720

(415) 486-5600

Robert J. Birgeneau
Mass. Institute of Technology
Department of Physics
Room 13-2114
Cambridge, MA 02139

(617) 253-4937

Gregory S. Blackman
MMRD, Building 62
Lawrence Berkeley Laboratory
Berkeley, CA 94720

(415) 486-5600

Richard J. Blake
SERC Daresbury Laboratory
Daresbury, Warrington
Cheshire WA4 4AD
ENGLAND

0925 65000

Charles Bonapace
Princeton University
Department of Electrical
Engineering & Computer Science
Princeton, NJ 08544

(609) 452-4642

Alexander M. Bradshaw
Fritz-Haber Institute
Faradayweg 4-6
1000 Berlin 33
WEST GERMANY

(30) 83 05 501

Ross D. Bringans
Xerox P.A.R.C.
3333 Coyote Hill Road
Palo Alto, CA 94304

(415) 494-4156

Hans-Joachim R. Brocksch
Freie Universitat Berlin
FB20 WE 05
Arnimallee 14
D-1000 Berlin 33, W. GERMANY

Eric Bullock
2545 The Mall
University of Hawaii
Honolulu, HI 96822

(808) 948-7380

Gianluigi Casalone
University of Milano
Dipartimento di Chimica Fisica
Via Golgi 19
Milano 20133, ITALY

(02) 292900

Yves J. Chabal
AT&T Bell Laboratories
600 Mountain Avenue, MH1C-333
Murray Hill, NJ 07974

(201) 582-4193

D. J. Chadi
Xerox, Palo Alto Research Center
3333 Coyote Hill Road
Palo Alto, CA 94304

(415) 969-4499

Chi Ming Chan
Raychem Corporation
300 Constitution Drive
Menlo Park, CA 94025

(415) 361-5351

Cheng-Hsuan Chen
AT&T Bell Laboratories
600 Mountain Avenue
Murray Hill, NJ 07974

(201) 582-7923

Shirley Chiang
IBM Research Laboratory
K33/281, 5600 Cottle Road
San Jose, CA 95193

(408) 256-7318

Pietro Chiaradia
CNR - Italy
Via E. Fermi 38
Frascati, Rome 00044

(06) 9426335

Paul H. Citrin
AT&T Bell Laboratories
100 Mountain Avenue
Murray Hill, NJ 07974

(201) 582-5275

Marvin L. Cohen
University of California-Berkeley
Department of Physics
Berkeley, CA 94720

(415) 642-4753

Philip I. Cohen
University of Minnesota
123 Church Street, SE
Minneapolis, MN 55455

(612) 373-2577

Warren Eugene Collins
Southern University
Baton Rouge, LA 70813

(504) 771-4130

Edward H. Conrad
University of Washington
BG-10, Chemistry Department
Seattle, WA 98185

(206) 545-2594

Matthew W. Copel
Department of Physics
University of Pennsylvania
209 South 33rd Street
Philadelphia, PA 19104

(215) 898-7943

Renee D. Diehl
University of Liverpool
Department of Physics
Oliver Lodge Laboratory
Liverpool L69 3BX, ENGLAND

(051) 709-6022, ext. 2247

Charles B. Duke
Xerox Webster Research Center
800 Phillips Road, 114
Webster, NY 14580

(716) 422-2109

Juergen Eckert
Los Alamos National Laboratory
Mail Stop H 805, P-8
Los Alamos, NM 87545

(505) 667-6069

William F. Egelhoff, Jr.
Surface Science Division
National Bureau of Standards
Gaithersburg, MD 20899

(301) 921-2788

Adolfo G. Equiluz
University of California-Irvine
Department of Physics
Irvine, CA 92717

(714) 856-6250

Gert Ehrlich
Coordinated Science Laboratory
University of Illinois
1101 West Springfield Avenue
Urbana, IL 61801

(217) 333-6448

M. El-Batanouny
Boston University
590 Commonwealth Avenue
Boston, MA 02215

(617) 353-4721

Charles S. Fadlem
Chemistry Department
2545 The Mall
University of Hawaii
Honolulu, HI 96822

(808) 948-6401

Sam Fain
University of Washington
Physics Department
Seattle, WA 98195

(206) 543-5729

L. M. Falicov
Department of Physics
University of California
Berkeley, CA 94720

(415) 642-5993

Helen H. Farrell
Bell Communications Research
600 Mountain Avenue
Murray Hill, NJ 07928

(201) 582-3791

T. E. Felter
Sandia
Livermore, CA 94550

(415) 443-7399

Salvador Ferrer
Univ. Auton. of Madrid
Cantoblanco
Madrid 34
SPAIN

734-0100, ext. 1758

William Fink
Department of Chemistry
University of California-Davis
Davis, CA 95616

(916) 753-5717

Michael Fluss
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60514

(312) 972-5149

Stephen M. Foiles
Sandia National Laboratories
Livermore, CA 94596

(415) 422-2898

Robert F. Frindt
Physics Department
Simon Fraser University
Burnaby, BC V5A 1S6, CANADA

(604) 291-3161 or 291-3703

Paul H. Fuoss
AT&T Bell Laboratories
4B415, Crawford's Corner Road
Holmdel, NJ 07733

(201) 949-3581

Eric Garfunkel
Rutgers University
New Brunswick, NJ 08903

Stephen H. Garofalini
Rutgers University
Department of Ceramics
P.O. Box 909
Piscataway, NJ 08854

(201) 932-2216

Edward L. Garwin
Stanford Linear Accelerator Center
P. O. Box 4349, Bin 72
Stanford, CA 94305

(415) 854-3300, ext. 2415

Jack G. Gay
General Motors Research Labs.
Physics Department
Warren, MI 48090-9055

(313) 575-2898

Walter M. Gibson
State University of N.Y.-Albany
Department of Physics
1400 Washington Avenue
Albany, NY 12722

(518) 457-8305

Rex W. Godby
Cavendish Laboratory
Madingley Road
Cambridge CB2 1RF
ENGLAND

(0223) 66477, ext. 415

Torgny Gustafsson
University of Pennsylvania
Philadelphia, PA 19104

(215) 898-5953

Jochen Haase
Fritz-Haber Inst. der MPG
4-6 Faradayweg
1000 Berlin 33
WEST GERMANY

Timur Halicioğlu
Stanford University (ELORET)
Stanford, CA 94305

(415) 497-3268

Burl M. Hall
Department of Physics
University of California-Irvine
Irvine, CA 92717

(714) 856-5453

Donald R. Hamann
AT&T Bell Laboratories
600 Mountain Avenue
Murray Hill, NJ 07974

(201) 582-4454

Dan Haneman
University of New South Wales
School of Physics
P. O. Box 1
Kensington, NSW 2033
AUSTRALIA

Martin Henzler
Institut für Festkörperphysik,
Universität
Appelstr. 2
3000 Hannover, WEST GERMANY

49-511-762-4821

Frank Herman
IBM Research Laboratory K32/281
5600 Cottle Road
San Jose, CA 95193

(408) 256-6254

Kai-Ming Ho
Ames Laboratory, Physics Dept.
Iowa State University
Ames, IA 50011

(515) 294-1960; 294-7712

R. Howell
Lawrence Livermore National Lab.
Livermore, CA 94550

(415) 422-1977

Tung Hsu
Arizona State University
Department of Physics
Tempe, AZ 85287

(602) 965-3561

Gen-you Hu
Physics Department
Brown University
Providence, RI 02912

Harald Ibach
IGV/KFA Julich
Postfach 1913
D-5170 Julich
WEST GERMANY

2461/614561

Alex Ignatiev
University of Houston
Department of Physics
University Park
Houston, TX 77004

(713) 749-3889

Jisoon Ihm
Bell Communications Research
65 Tussel Lane
Scotch Plains, NJ 07076

(201) 582-2884

Thomas E. Jackman
Chalk River Nuclear Laboratories
Solid State Science
Chalk River, Ontario K0J 1J0
CANADA

(613) 584-3311 ext. 2357

Les Jenkins
Oak Ridge National Laboratory
Building 3025, P. O. Box X
Oak Ridge, TN 37831

A. Norman Jette
The Johns Hopkins Univ.
Applied Physics Laboratory
Johns Hopkins Road
Laurel, MD 20707

(301) 953-6263

John D. Joannopoulos
Massachusetts Inst. of Technology
77 Massachusetts Avenue, 12-116
Cambridge, MA 02139

(617) 253-4806

Robert L. Johnson
Max-Planck Institut
Heisenbergstr. 1
D-7000 Stuttgart 80
WEST GERMANY

0711 6860 626

Franco P. Jona
State University of New York
Department of Materials Science
Stony Brook, NY 11794

(516) 246-7649

Donald S. Kaufman
University of Washington
BG-10, Department of Chemistry
Seattle, WA 98195

(206) 545-2954

Efthimios Kaxiras
Massachusetts Inst. of Technology
77 Massachusetts Avenue
Room 12-128B
Cambridge, MA 02139

(617) 253-5947

Robert E. Kirby
Stanford Linear Accelerator Center
Mail Stop 74
P.O. Box 4349
Stanford, CA 94305

(415) 854-3300, ext. 2795

Ondrej L. Krivanek
Center for Solid State Science
Arizona State University
Tempe, AZ 85287

(602) 965-7512

Jean C. Lapujoulade
CEN Saclay DPhG-PAS
GIF sur Yvette Cedex 91191
FRANCE

(6) 908-25-33

Le Lay
CNRS - CRNCZ
Campus de Luminy Case 913
Marseille
FRANCE

Keum H. Lee
University of Missouri
Department of Physics
Columbia, MO 65211

(314) 882-6735 or 882-3434

Steven Levine
Rutgers University
Brett Road
Biscataway, NJ 08854

(201) 932-2216

Joe C. H. Li
Microlinear
San Jose, CA

(408) 262-5200, ext. 535

Keng-San Liang
Exxon Research & Engineering Co.
Rt. 22 East, Clinton Township
Annandale, NJ 08801

(201) 730-3032

Ingolf Lindau
Stanford University
Stanford Electronics Laboratories
Stanford, CA 94305

(415) 497-1052

Frederick W. Lipps
University of Houston, Energy Lab.
4801 Calhoun St., Bldg. SPA
Houston, TX 77004

(713) 749-1155

Gu Liu
Lawrence Berkeley Laboratory
1 Cyclotron Road, 70A-1115
Berkeley, CA 94720

(415) 486-5666

Steven G. Louie
University of California
Department of Physics
Berkeley, CA 94720

(415) 642-1709

Theodore E. Madey
National Bureau of Standards
Chemistry Building, Room B248
Washington, DC 20234

(301) 921-2188

Robert J. Madix
Stanford University
Department of Chemical Engineering
Stauffer III
Stanford, CA 94305

(415) 497-2402 or 497-4906

Richard G. Masters
Harris Semiconductor
Analytical Services Dept.
P.O. Box 883, M.S. 62-007
Melbourne, FL 32901

(305) 724-7283

C. Mathew Mate
MMRD, Building 62
Lawrence Berkeley Laboratory
Berkeley, CA 94720

(415) 486-5600

E. G. McRae
AT&T Bell Laboratories
Murray Hill, NJ 07974

(201) 582-4738

Michael J. Mehl
Sachs Freeman Associates
c/o Naval Research Laboratory
Code 6684
Washington, DC 20735

(202) 767-3934

Eugene C. Mele
University of Pennsylvania
Department of Physics
Philadelphia, PA 19104

(215) 898-3135

P. Meyer
Lawrence Livermore National Lab.
P.O. Box 808
Livermore, CA 94550

(415) 422-9678

Christian J. Minot
Universite de Paris-Sud
Orsay, 91405 FRANCE

33(6) 941-61-75

Winfried Monch
University of Duisburg
Bismarckstr. 81
D-4100 Duisburg
WEST GERMANY

(0203) 379-3265

Hans Morawitz
IBM Research Lab, Department K33
5600 Cottle Road
San Jose, CA 95193

(408) 256-2174

Raymond Moreh
Ben-Gurion University of Negev
Physics Department
Beer-Sheva 84120
ISRAEL

Bernard J. Mrstik
Naval Research Laboratory
Code 6834
Washington, DC 20375

(202) 767-3414

Klaus E. Muller
University of Erlangen
Erwin-Rommel-Str. 1
Lehrstuhl fur
Festkorperphysik
Erwin-Rommel-Str. 1
D8520 Erlangen, WEST GERMANY

Lee E. Myers
USAF Office of Scientific Research
AFOSR/NC
Bolling AFB, DC 20332

(202) 767-4963

Seido Nagano
Univ. of Wisconsin-Milwaukee
Milwaukee, WI 53211

(414) 963-4969

Connie J. Nelin
Analatom Inc
253 Humboldt Court
Sunnyvale, CA 94082

(415) 965-6231

Jacqueline M. Nicol
University of Durham, UK
c/o Los Alamos Nat'l Laboratory
Mail Stop H805
Los Alamos, NM 87545

(505) 667-6069

Osamu Nishikawa
Tokyo Institute of Technology
Dept. of Mat. Sci. & Eng.
4259 Nagatsuta, Midori-ku
Yokohama 227, JAPAN

(045) 922-1111 Ext. 2621

John Noonan
Oak Ridge National Laboratory
Building 3025 - P. O. Box X
Oak Ridge, TN 37831

Peter J. A. Nordlander
Chalmers University
S-412 96 Gothenburg
SWEDEN

David Norman
Daresbury Laboratory
S.E.R.C.
Warrington WA4 4AD
UNITED KINGDOM

(925) 65000

Jens K. Norskov
NORDITA
Blegdamsvej 17
DK-2100 Copenhagen
DENMARK

(1) 421616

John E. Northrup
Xerox, Palo Alto Research Center
3333 Coyote Hill Road
Palo Alto, CA 94304

(415) 494-4187

David F. Ogletree
MMRD, Building 62
Lawrence Berkeley Laboratory
Berkeley, CA 94720

(415) 486-6067

Marjorie A. Olmstead
Lawrence Berkeley Laboratory
Bldg. 70, Rm. 110
Berkeley, CA 94720

(415) 486-5809

John Osen
University of Washington
Physics Department
Seattle, WA 98195

(206) 543-5729

Steven H. Overbury
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

(615) 574-5040

Juan Parellada-Sabata
Facultat de Fisica
Universitat de Barcelona
Diagonal 645
Barcelona 28, SPAIN

(343) 330.73.11 ext 242

Bradford B. Pate
SSRL, Stanford University
SLAC Bin 69, PO Box 4349
Stanford, CA 94305

(415) 854-3300 x3445

John B. Pendry
Imperial College
Department of Physics
Prince Consort Road
London SW7 2BZ, ENGLAND

(01) 589-5111, ext 2304

Piero Pianetta
Stanford University
SLAC - Bin 69
P.O. Box 4349
Stanford, CA 94305

(415) 854-3300, ext. 3484

Joseph Pimbley
General Electric/RPI
15 Cheshire Place
Schenectady, NY 12309

(518) 393-0890

Fernando A. Ponce
Xerox Palo Alto Research Center
3333 Coyote Hill Road
Palo Alto, CA 94304

(415) 494-4199

Hin Chuck Poon
Univ. of Wisconsin-Milwaukee
Milwaukee, WI 53201

(414) 963-6082

Paul Pukite
University of Minnesota
123 Church Street, SE
Minneapolis, MN

(612) 373-2482

Neville Vincent Richardson
University of Liverpool
Donnan Labs., Grove Street
Liverpool L69 3BX
UNITED KINGDOM

051-709-6022, ext. 2560

Steven L. Richardson
Department of Physics
Univ. of California at Berkeley
Berkeley, CA 94720

(415) 642-1031, or 642-4753

Roy Richter
General Motors Research Labs.
Physics Department
Warren, MI 48090-9055

(313) 575-2901

Ian K. Robinson
Bell Laboratories
Murray Hill, NJ 07974

(201) 582-6056

Lyle D. Roelofs
University of Maryland
Department of Physics & Astronomy
College Park, MD 20742

(301) 454-7043

Ira J. Rosenberg
Lawrence Livermore National Lab.
Livermore, CA 94550

(415) 422-0684

Gerd M. Rosenblatt
Chemistry Division
Los Alamos National Laboratory
CHM-DO, MS J563
Los Alamos, NM 87545

(505) 667-6250

Gianfranco Rovida
Dipartimento di Chimica
Via G. Capponi 9
50121 Firenze
ITALY

240865

Jack E. Rowe
Physics Department
University of Florida
Gainesville, FL 32611

(904) 392-0521 - (904) 392-7334

Jack E. Rowe
University of Florida
Department of Physics
Gainesville, FL 32611

(904) 392-7334 or 0521

Takasi Sagawa
Tohoku University
Department of Physics
Sendai 980
JAPAN

0222-22-1800, ext. 3239

Dilano K. Saldin
Imperial College of Science
and Technology
Prince Consort Road
London SW7 2BZ, ENGLAND

(01) 589-5111

Lionel Salem
Centre d'Orsay
Universite de Paris-Sud
Lab. de Chimie Theorique
91405 Orsay
FRANCE

David A. Saloner
University of Wisconsin-Madison
Materials Science Program
1111 ERB, 1500 Johnson Drive
Madison, WI 53706

(608) 263-2089

Robert Schlogl
University of Basle
Ulingelsergstr. 82
CH 4056 Basle
SWITZERLAND

Matthias Schoebinger
IBM San Jose/ K33-281
5600 Cottle Road
San Jose, CA 95193

(408) 256-2190

Claude A. Sebenne
Lab Physique des Solides
Universite P. et M. Curie
4 Place Jussieu
75230 Paris CEDEX 05
FRANCE

Annabella Selloni
Department of Physics
University of Rome
P22a A. Moro, 2
00185 Roma
ITALY

Massimo Simonetta
University of Milan
Via Golgi 19
20122 Milano
ITALY

2/292900

Charles P. Slichter
University of Illinois at Urbana
1110 W. Green Street
Urbana, IL 61801

(217) 333-3834

Leon Smit
FOM Institute for Atomic and
Molecular Physics
P.O. Box 41883
1009 DB Amsterdam
THE NETHERLANDS

John R. Smith
General Motors Research
Physics Department
Warren, MI 98090-9055

(313) 575-2826

Gabor A. Somorjai
University of California
Department of Chemistry
Berkeley, CA 94720

(415) 642-4053

William E. Spicer
Stanford University
Stanford Electronics Laboratories
McCullough Building #228
Stanford, CA 94305

(415) 497-4643

John L. Stickney
University of California
at Santa Barbara
Santa Barbara, CA 93106

(805) 961-3905

Joachim Stohr
Exxon Research & Engineering Co.
Annandale, NJ 08801

(516) 282-2070

Masaetsu Takahashi
#863 I House,
2299 Piedmont Avenue
Berkeley, CA 94720

(415) 643-3052

Takashi Takahashi
Tohoku University
Department of Physics
Sendai 980
JAPAN

0222-22-1800, ext. 3239

Tadayoshi Takai
Material Science and Engineering
Stanford University
Stanford, CA 94305

(415) 497-9497

Ariadne Tenner
FOM-Institute for Atomic and
Molecular Physics
Kruislaan 407
1098 SJ Amsterdam
THE NETHERLANDS

Jerry D. Tersoff
AT&T Bell Laboratories
600 Mountain Avenue, Room 7C325
Murray Hill, NJ 07974

(201) 582-7350

Patricia A. Thiel
Iowa State University
Ames, IA 50011

(515) 294-8985

Hiroshi Tochihara
The University of Tokyo
Institute for Solid State Physics
Roppongi 7-22-1, Minato-ku
Tokyo 106, JAPAN

3-476-6811 ext. 5302

David Tomanek
Freie Universitat Berlin, FB Physik
Arnimallee 14
Berlin 33 D-1000
WEST GERMANY

(030) 838-3797

David S. Y. Tong
Univ. of Wisconsin - Milwaukee
P.O. Box 413
Milwaukee, WI 53201

(414) 351-1389 or 963-4474

Ruud M. Tromp
IBM
Thomas J. Watson Research Center
P. O. Box 218
Yorktown Heights, NY 10598

(914) 945-1242

Tien T. Tsong
Pennsylvania State University
104 Davey Laboratory
University Park, PA 16802

(814) 865-2813

Roger Uhrberg
Xerox, Palo Alto
3333 Coyote Hill Road
Palo Alto, CA 94304

(415) 494-4181

Cyrus J. Umrigar
Cornell University
Clark Hall - LASSP
Ithaca, NY 14850

(607) 256-6487

William N. Unertl
LASST, 2 Barrows Hall
University of Maine
Orono, ME 04469

(207) 581-2251

Thomas Upton
Exxon Research & Engineering
Rt. 22 East
Annandale, NJ 08801

(201) 730-2555

Jan H. van der Merwe
University of Pretoria
Pretoria 0002, Transvaal
SOUTH AFRICA

(012) 420 2459

Michel A. Van Hove
MMRD, Building 62
Lawrence Berkeley Laboratory
Berkeley, CA 94720

(415) 486-6160

David Vanderbilt
University of California
Department of Physics
Berkeley, CA 94720

(415) 642-1031

Randall H. Victora
Department of Physics
University of California
Berkeley, CA 94720

(415) 642-5993

Arthur J. Viescas
Stanford University
251 McCullough - SEL
Stanford, CA 94086

(415) 497-3209

Dennis T. Vigen
University of the Saar
Inst. fur Theor. Physik
6600 Saarbrücken
WEST GERMANY

(681) 302-3967

Ching-Ping S. Wang
Department of Physics
University of Maryland
College Park, MD 20742

(301) 454-6628

Po-Kang Wang
University of Illinois-Urbana
Department of Physics
1110 W. Green Street
Urbana, IL 61801

(217) 333-4628

Sheng-Wei Wang
Lawrence Berkeley Laboratory
1 Cyclotron Road
Berkeley, CA 94720

(415) 486-4821

Xun Wang
Physics Department
Fudan University
Shanghai
PEOPLE'S REPUBLIC OF CHINA

480906, ext. 172

Maurice B. Webb
University of Wisconsin-Madison
Physics Department
Madison, WI 53705

(608) 233-6797

Jerry L. Whitten
S.U.N.Y. at Stony Brook
Chemistry Department
Stony Brook, NY 11794

(516) 246-6068

R. Stanley Williams
Univ. of Calif. at Los Angeles
Department of Chemistry
Los Angeles, CA 90024

(213) 825-8818

Roy F. Willis
Cavendish Laboratory
Department of Physics
Madingley Road
Cambridge CB3 0HE
ENGLAND

R. J. Wilson
IBM Research
5600 Cottle Road
San Jose, CA 95193

(408) 256-2491

Christopher J. Wright
A.E.R.E. Harwell
Building 521
Didcot, Oxon. OX110RA
ENGLAND

(0235) 21054, ext. 5208

Naijuan Wu
University of Houston
Department of Physics
Houston, TX

Xide Xie
Physics Department
Fudan University
Shanghai
PEOPLE'S REPUBLIC OF CHINA

480906, ext. 172, 483331

Mu-Liang Xu
Univ. of Wisconsin - Milwaukee
Milwaukee, WI 53201

(414) 963-6082

Chia H. Yang
Southern University
Baton Rouge, LA 70813

(504) 771-4130

W. S. Yang
Peking University
Beijing
CHINA

Jory Yarnoff
UCLA, Chemistry Department
405 Hilgard Avenue
Los Angeles, CA 90024

(213) 206-8393

See-Chen Ying
Brown University
Providence, RI 02912

(401) 863-2684

Hoydoo You
University of Washington
Physics Department
Seattle, WA 98195

(206) 543-5729

Shengbai Zhang
University of California-Berkeley
Department of Physics
Berkeley, CA 94720

(415) 642-2635

Paul R. Zschack
Northwestern University
2145 Sheridan Road
Evanston, IL 60201

(312) 492-7677