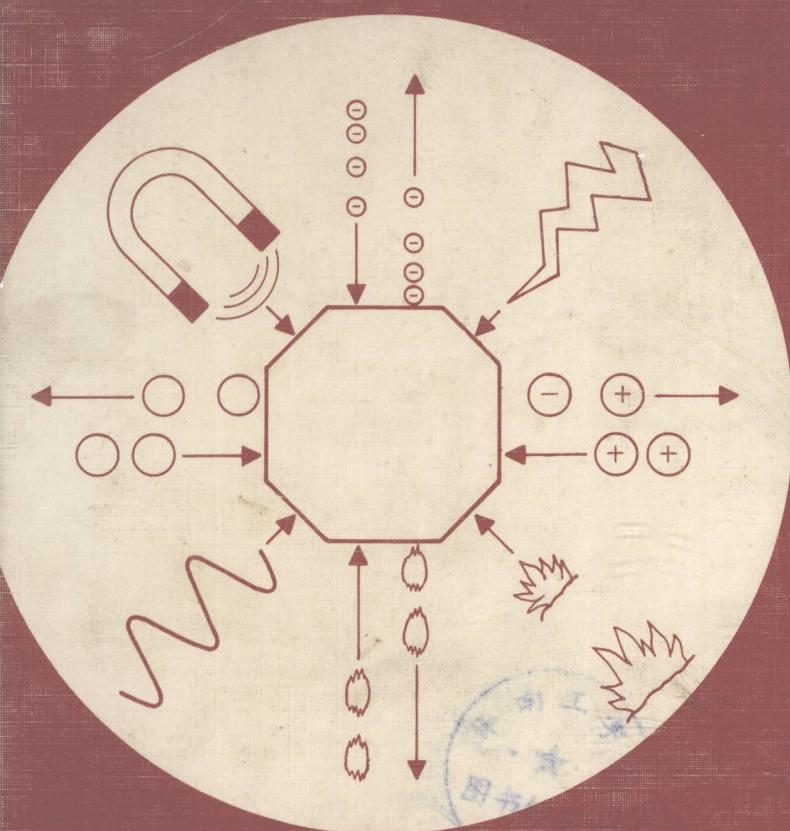


**studies in surface science and catalysis**

**14**



# VIBRATIONS AT SURFACES

**C.R. Brundle**  
and  
**H. Morawitz**  
(editors)

**elsevier scientific publishing company**

0647.1

BI

8461057

8461057

Studies in Surface Science and Catalysis 14

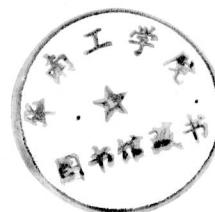
# VIBRATIONS AT SURFACES

Proceedings of the Third International Conference,  
Asilomar, California, U.S.A., 1–4 September 1982

Editors

C.R. BRUNICLE and H. MORAWITZ

IBM Research, 5600 Cottle Road, San José, CA 95193, U.S.A.



Reprinted from the *Journal of Electron Spectroscopy and Related Phenomena*,  
Volumes 29 (Part A) and 30 (Part B)



ELSEVIER SCIENTIFIC PUBLISHING COMPANY  
Amsterdam – Oxford – New York 1983

TOP SECRET

ELSEVIER SCIENTIFIC PUBLISHING COMPANY  
Molenwerf 1,  
P.O. Box 211, 1000 AE Amsterdam, The Netherlands

*Distributors for the United States and Canada:*

ELSEVIER SCIENCE PUBLISHING COMPANY INC.  
52, Vanderbilt Avenue  
New York, N.Y. 10017

ISBN 0-444-42166-1 (Vol. 14)  
ISBN 0-444-41801-6 (Series)

© Elsevier Science Publishers B.V., 1983

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise without the prior written permission of the publisher, Elsevier Science Publishers B.V., P.O. Box 330, 1000 AH Amsterdam, The Netherlands.

Printed in The Netherlands

**Studies in Surface Science and Catalysis 14**

**VIBRATIONS AT SURFACES**

## Studies in Surface Science and Catalysis

- Volume 1 **Preparation of Catalysts I.** Scientific Bases for the Preparation of Heterogeneous Catalysts. Proceedings of the First International Symposium held at the Solvay Research Centre, Brussels, October 14–17, 1975  
edited by **B. Delmon, P.A. Jacobs and G. Poncelet**
- Volume 2 **The Control of the Reactivity of Solids.** A Critical Survey of the Factors that Influence the Reactivity of Solids, with Special Emphasis on the Control of the Chemical Processes in Relation to Practical Applications  
by **V.V. Boldyrev, M. Bulens and B. Delmon**
- Volume 3 **Preparation of Catalysts II.** Scientific Bases for the Preparation of Heterogeneous Catalysts. Proceedings of the Second International Symposium, Louvain-la-Neuve, September 4–7, 1978  
edited by **B. Delmon, P. Grange, P. Jacobs and G. Poncelet**
- Volume 4 **Growth and Properties of Metal Clusters.** Applications to Catalysis and the Photographic Process. Proceedings of the 32nd International Meeting of the Société de Chimie physique, Villeurbanne, September 24–28, 1979  
edited by **J. Bourdon**
- Volume 5 **Catalysis by Zeolites.** Proceedings of an International Symposium organized by the Institut de Recherches sur la Catalyse – CNRS – Villeurbanne and sponsored by the Centre National de la Recherche Scientifique, Ecully (Lyon), September 9–11, 1980  
edited by **B. Imelik, C. Naccache, Y. Ben Taarit, J.C. Vedrine, G. Coudurier and H. Praliaud**
- Volume 6 **Catalyst Deactivation.** Proceedings of the International Symposium, Antwerp, October 13–15, 1980  
edited by **B. Delmon and G.F. Froment**
- Volume 7 **New Horizons in Catalysis.** Proceedings of the 7th International Congress on Catalysis, Tokyo, 30 June–4 July 1980  
edited by **T. Seiyama and K. Tanabe**
- Volume 8 **Catalysis by Supported Complexes**  
by **Yu.I. Yermakov, B.N. Kuznetsov and V.A. Zakharov**
- Volume 9 **Physics of Solid Surfaces.** Proceedings of the Symposium held in Bechyňe, Czechoslovakia, September 29–October 3, 1980  
edited by **M. Láznička**
- Volume 10 **Adsorption at the Gas–Solid and Liquid–Solid Interface.** Proceedings of an International Symposium held in Aix-en-Provence, September 21–23, 1981  
edited by **J. Rouquerol and K.S.W. Sing**
- Volume 11 **Metal-Support and Metal-Additive Effects in Catalysis.** Proceedings of an International Symposium organized by the Institut de Recherches sur la Catalyse – CNRS – Villeurbanne and sponsored by the Centre National de la Recherche Scientifique, Ecully (Lyon), September 14–16, 1982  
edited by **B. Imelik, C. Naccache, G. Coudurier, H. Praliaud, P. Meriaudeau, P. Gallezot, G.A. Martin and J.C. Vedrine**
- Volume 12 **Metal Microstructures in Zeolites.** Preparation – Properties – Applications.  
Proceedings of a Workshop, Bremen, September 22–24, 1982  
edited by **P.A. Jacobs, N.I. Jager, P. Jiru and G. Schulz-Ekloff**
- Volume 13 **Adsorption on Metal Surfaces.** An Integrated Approach  
edited by **J. Bénard**
- Volume 14 **Vibrations at Surfaces.** Proceedings of the Third International Conference, Asilomar, California, U.S.A., 1–4 September 1982  
edited by **C.R. Brundle and H. Morawitz**

## **FOREWORD**

The third International Conference on " Vibrations at Surfaces " (VAS III) was held at Asilomar, California, from September 1-4, 1982. It followed its two forerunners held in Juelich, West Germany in 1978 and Namur, Belgium in 1980 with clear indications of continuing and increasing growth in both experimental and theoretical activities, sophistication and understanding.

Almost all of the 102 papers presented at the meeting are published in this volume. A few papers appear as abstracts only due to prior commitment to other publication channels or choice of authors and/or editors.

The conference attracted about 165 participants active in the field, and was organized by a group of scientists from the IBM Research Laboratory in San Jose, California acting as local committee. The hard-working members of this group included:

D. Auerbach	F. Houle
P. Bagus	A. Luntz
J. Barker	H. Morawitz (Chairman)
I. Batra	M. Philpott
R. Brundle	J. Rabolt
T. Chuang	H. Seki
F. Herman	J. Swalen

To cover the range of work relevant to the theme of the meeting, a set of eight session topics were chosen with the help of an International Advisory Committee consisting of :

S. Anderson, Sweden	B. Lundquist, Sweden
G. Boato, Italy	D. Menzel, Germany
E. Burstein, U.S.A.	A. Otto, Germany
C. Imbert, France	J. E. Rowe, U.S.A.
H. Ibach, Germany	W. Suetaka, Japan
D. King, England	P. Toennies, Germany
J. Kirtley, U.S.A.	R. Van Duyne, U.S.A.
A. Lucas, Belgium	H. Weinberg, U.S.A.

The topics chosen for the eight sessions held over a span of 3 days were: (I) Vibrational Frequency Shifts and Widths-Lateral Interactions; (II) Dynamical Processes at Surfaces; (III) and (IV) Electron Loss Spectroscopy; (V) Raman and Surface Enhanced Raman Scattering; (VI) Infrared Absorption and Reflection Spectroscopy; (VII) Beam Surface Scattering - Surface Phonons; (VIII) Electron Tunnelling Spectroscopy - Surface Enhanced Raman Studies in Electrochemistry. In addition, C. B. Duke presented an introductory keynote surveying progress in the field since the last meeting. In the final session H. Ibach and T. Grimley presented conference overviews and future prospects for the field from an experimental and theoretical perspective.

Also included in the Proceedings are four literature surveys on Energy Loss, Inelastic Tunnelling, Infrared and Raman (SERS) papers. The ones on EELS and Infrared are updates of similar surveys appearing in the Proceedings of VAS II, the remaining two are new additions.

A striking aspect of the meeting was the presence of much work related to dynamical effects occurring in atom and molecule-surface interactions. While the static properties of both surface and adsorbate define the zero order response, it is clear that many of the techniques used and properties determined in vibrational surface spectroscopy in fact depend on dynamical changes in both surface and adsorbate behavior. Typical examples are the various enhancement mechanisms proposed in SERS, the effect of substrate phonon and electronic excitations in atom and molecule scattering experiments and the interplay of local and collective modes in overlayer vibrations to mention a few.

The conference proved the timeliness of a two year period and provided a convenient geographical locus for the Pacific sector of surface vibrational spectroscopy given the European locations of VAS I and II. The conference organizers gratefully acknowledge generous support from the IBM Research Laboratory at San Jose, the National Science Foundation, the Air Force Office of Scientific Research, The Office of Naval Research, the International Union of Pure and Applied Physics and the American Physical Society for sponsorship and financial aid. Finally, Mrs. Beth MacQuiddy as conference secretary did a superb job keeping track of the myriad of logistical details and deserves the full gratitude of the organizing committee and all participants.

C. R. Brundle and H. Morawitz

(Guest Editors)

VIBRATIONS AT SURFACES CONFERENCE  
September 1-4, 1982

Registered Participants

- Frank J. Adrian  
Johns Hopkins University/APL  
Laurel, MD 20707
- Paul Alivisatos  
Chemistry Department  
University of California  
Berkeley, CA 94720
- Guy Allan  
Bell Laboratories  
600 Mountain Avenue  
Murray Hill, NJ 07974
- D. Allara  
Bell Laboratories  
600 Mountain Avenue  
Murray Hill, NJ 07974
- Brad Anton  
California Institute of Technology  
208-41  
Pasadena, CA 91125
- D. Auerbach  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193
- Neil Avery  
CSIRO Div. of Materials Sci.  
University of Melbourne  
Parkville, Victoria 3052  
AUSTRALIA
- Phaedon Avouris  
IBM Research Center  
Yorktown Heights, NY 10598
- Albert G. Baca  
Bldg 70A-1117  
Lawrence Berkeley Laboratory  
Berkeley, CA 94720
- Simon R. Bare  
Department I.P.I Chemistry  
University of Liverpool  
Mereyside L59 3BX, Liverpool  
ENGLAND
- John A. Barker  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193
- Inder P. Batra  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193
- Christopher H. Becker  
SRI International  
Molecular Physics Laboratory  
333 Ravenswood Dr.  
Menlo Park, CA 94025
- Hans-Ottman Beckmann  
Department of Chemistry  
SUNY at Stony Brook  
Stony Brook, NY 11794
- Giorgio Benedek  
Ist. di Fisica  
V. Celoria 16  
I-2-133 Milano, ITALY
- Richard C. Benson  
Johns Hopkins University/APL  
Johns Hopkins Road  
Laurel, MD 20707
- Steven L. Bernasek  
Department of Chemistry  
Princeton University  
Princeton, NJ 08544
- J. Black  
17 Valerie  
L1T 3G3 St. Catharines  
CANADA
- C. Richard Brundle  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

Donald Burgess  
Department of Chemistry  
Northwestern University  
Evanston, IL 60201

Elias Burstein  
Physics Department  
University of Pennsylvania  
Philadelphia, PA 19104

Alan Campion  
Department of Chemistry  
University of Texas  
Austin, TX 78712

M. Casassa  
California Institute of Technology  
127-72  
Pasadena, CA 91125

Richard Cavanagh  
B-268 Physics  
National Bureau of Standards  
Washington, DC 20234

Francis Celii  
California Institute of Technology  
127-72  
Pasadena, CA 91125

Yves J. Chabal  
Bell Laboratories  
600 Mountain Avenue, MH2D-318  
Murray Hill, NJ 07974

M. A. Chesters  
School of Chemical Sciences  
University of East Anglia  
Norwich NR4 7TJ  
UNITED KINGDOM

Shirley Chiang  
Department of Physics  
University of California  
Berkeley, CA 94720

Chih-Cong Chou  
Department of Chemistry  
University of California  
Irvine, CA 92717

Tung J. Chuang  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

P. Anthony Cox  
Inorganic Chemistry Laboratory  
South Parks Road  
Oxford OX1 3QR, ENGLAND

Jon B. Cross  
Los Alamos National Laboratory  
CNC-2, MS 732  
Los Alamos, NM 87545

John E. Crowell  
Department of Chemistry  
University of California  
Berkeley, CA 94720

B. M. Davies  
Department of Chemistry  
University of Texas  
Austin, TX 78712

J. E. Demuth  
IBM Research Center  
Yorktown Heights, NY 10598

F. W. DeWette  
Department of Physics  
University of Texas  
Austin, TX 78712

R. E. Dietz  
Bell Laboratories  
600 Mountain Avenue  
Murray Hill, NJ 07974

Rolf Dornhaus  
Kruppstr. 6  
D-5100 Aachen 1  
WEST GERMANY

Lawrence H. Dubois  
Bell Laboratories  
600 Mountain Avenue, 1A-280  
Murray Hill, NJ 07974

Charles Duke  
Xerox Webster Research Ctr.  
Bldg. 114  
Rochester, NY 14644

Hardouin Duparc  
c/o A. A. Maradudin  
Department of Physics  
University of California  
Irvine, CA 92717

Gary L. Eesley  
Physics Department  
GM Research Laboratory  
Warren, MI 48090

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

Thomas Engel  
Department of Chemistry  
University of Washington  
Seattle, WA 98195

Wulf Erley  
KFA/IGV  
5270 Juelich  
WEST GERMANY

James L. Erskine  
Department of Physics  
University of Texas  
Austin, TX 78712

Galen Fisher  
Physical Chemistry Department  
General Motors  
Warren, MI 48090

John Freeman  
Monsanto Company  
800 N. Lindberg  
St. Louis, MO 67166

J. W. Gadzuk  
National Bureau of Standards  
Washington, DC 20234

Nicolas Garcia  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

S. Gauthier  
Groupe de Physique des  
solides de l'E.N.S.  
Tour 23, 2 place Jussieu  
75251 Paris, FRANCE

Steven George  
Department of Chemistry  
419 Latimer Hall  
University of California  
Berkeley, CA 94720

Nathaniel E. Glass  
Department of Physics  
University of California  
Irvine, CA 92717

W. A. Goddard III  
Department of Chemistry  
California Institute of Technology  
Pasadena, CA 91125

William Golden  
IBM A62/44  
San Jose, CA 95193

Gary Goncher  
Chemistry Department  
University of California  
Berkeley, CA 94720

Wolfgang Gopel  
Physics Department  
Montana State University  
Bozeman, MT 59717

Joseph G. Gordon  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

Robert Greenler  
Department of Physics  
University of Wisconsin  
Milwaukee, WI 53201

T. B. Grimley  
Donnan Laboratories  
University of Liverpool  
P. O. Box 147  
Liverpool L69 3BX  
UNITED KINGDOM

Paul Hansma  
Department of Physics  
University of California  
Santa Barbara, CA 93106

Bryan Hayden  
Fritz-Haber-Institut  
Faradayweg 416  
1 Berlin 33  
WEST GERMANY

**Joachim Heidberg**  
Institut Physik. Chemie  
D-3000 Hannover  
WEST GERMANY

**John C. Hemminger**  
Department of Chemistry  
University of California  
Irvine, CA 92717

**David Heskett**  
Department of Physics  
University of Pennsylvania  
Philadelphia, PA 19104

**K. W. Hipp**  
Department of Chemistry  
Washington State University  
Pullman, WA 99164

**Friedrich Hoffmann**  
Exxon Corp. 16-A029  
Linden, NJ 07036

**Bill Hopewell**  
IBM San Jose  
A57/044  
San Jose, CA 95193

**Frances A. Houle**  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

**Heinrich E. Hunziker**  
IBM Research Laboratory  
K34/281  
San Jose, CA 95193

**Jerry E. Hurst Jr.**  
Department of Chemistry  
Stanford University  
Stanford, CA 94305

**Ingo Hussla**  
Inst. Phys. Chemie A  
Collinstr. 3-3a  
3000 Hannover  
WEST GERMANY

**Jeffrey Hylden**  
Department of Chemistry  
University of Minnesota  
Minneapolis, MN 55414

**Harald Ibach**  
KFA Julich IGB  
D517 Julich  
WEST GERMANY

**Rolf P. Jaeger**  
2830 Malabar Dr.  
Santa Clara, CA 95051

**Kenneth C. Janda**  
California Institute of Technology  
127-72  
Pasadena, CA 91125

**L. L. Kesmodel**  
Physics Department  
Indiana University  
Bloomington, IN 47405

**David King**  
Physical Chemistry Department  
University of Liverpool  
Liverpool  
UNITED KINGDOM

**G. Kirczenow**  
Physics Department  
Boston University  
Boston, MA 02215

**John Kirtley**  
IBM Research Center  
Yorktown Heights, NY 10598

**Richard Knochenmuss**  
Chemistry Department  
Washington State University  
Pullman, WA 99164

**Bruce E. Koel**  
Department of Chemistry  
University of California  
Berkeley, CA 94720

**M. L. Koszykowski**  
Sandia National Laboratories  
Livermore, CA 94550

**Glenn D. Kubik**  
Department of Chemistry  
Stanford University  
Stanford, CA 94305

**Keiji Kunimatsu**  
Research Inst. Catalysis  
Hokkaido University  
Sapporo 060, JAPAN

**David K. Lambert**  
Physics Department  
GM Research Laboratory  
Warren, MI 48040

**C. R. Leavens**  
244-2270 Cotter's Cres.  
Ottawa, Ontario  
CANADA K1V 8Y6

**Ingolf Lindau**  
SLAC, Bin #69  
Stanford University  
Stanford, CA 94305

**B. H. Loo**  
Materials Research Laboratory  
SRI International  
Menlo Park, CA 94025

**John J. Low**  
Noyes Laboratory (127-72)  
California Institute of Technology  
Pasadena, CA 91125

**Alan Luntz**  
IBM Research Laboratory  
K34/281  
San Jose, CA 95193

**Lahmer Lynds**  
United Technologies Research  
East Hartford, CT 06108

**Beth Mac Quiddy**  
IBM Research Laboratory  
K31/281  
San Jose, CA 95193

**Robert J. Madix**  
Chemical Engineering Department  
Stanford University  
Stanford, CA 94305

**Ursula Mazur**  
Department of Chemistry  
Washington State University  
Pullman, WA 94164

**Michael R. McClellan**  
P. O. Box 969  
Livermore, CA 94550

**Gary McClelland**  
Chemistry Department  
Harvard University  
Cambridge, MA 02138

**David R. Miller**  
Department A.M.E.S., B-010  
University of California  
La Jolla, CA 92093

**D. L. Mills**  
Department of Physics  
University of California  
Irvine, CA 92717

**Hans Morawitz**  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

**Cherry Murray**  
Bell Laboratories  
600 Mountain Avenue, 1E-343  
Murray Hill, NJ 07974

**Lee Myers**  
Office of Naval Research  
Washington, DC 20332

**Ron Naaman**  
Weizmann Institute  
Isotopes Research Department  
Rehovot, ISRAEL

**Mourits Nielsen**  
Atomic Energy Commission  
Research Establishment Risø  
DK-4000 Roskilde, DENMARK

**Mitsuaki Nishijima**  
Department of Chemistry  
Faculty of Science  
Kyoto University  
Kyoto, JAPAN

**Abraham Nitzan**  
Department of Chemistry  
Northwestern University  
Evanston, IL 60201

Fabrizio Nizzoli  
Istituto di Fisica Universita  
Modena, ITALY 41100

Curt Nyberg  
Department of Physics  
Chalmers University of Technology  
S-412 96 Goteborg  
SWEDEN

Andreas Otto  
Physikalisches Institut III  
Universitat Dusseldorf  
4000 Dusseldorf  
WEST GERMANY

John Overend  
Department of Chemistry  
University of Minnesota  
107 Pleasant St. SE  
Minneapolis, MN 55455

J. F. Owen  
Yale University  
P. O. Box 2157, Yale Station  
New Haven, CT 06520

Craig Parsons  
Chemistry Department  
University of California  
Berkeley, CA 94720

B. N. Persson  
KFA Julich  
D-5170 Julich  
WEST GERMANY

M. Persson  
Institute of Theoretical Physics  
Goteborg S-41296  
SWEDEN

Bruno Pettinger  
Fritz Haber Institute M76  
Faradayweg 4-6  
1000 Berlin  
WEST GERMANY

Herbert Pfneuer  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

M. R. Philpott  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

Jean-Jacques Pireaux  
F.N.D.P.  
61, rue de Bruxelles  
5000 Namur, BELGIUM

Iven Pockrand  
Physikalisches Institut III  
Universitatsstr. 1  
D-400 Dusseldorf 1  
WEST GERMANY

John F. Rabolt  
IBM Research Laboratory  
K42/282  
San Jose, CA 95193

Heinz Raether  
Universitaet Hamburg  
Inst. fur Angewandte Physik  
Jungiusstrasse 11  
2 Hamburg 36, WEST GERMANY

Talat S. Rahman  
1829 Santa Ana Ave.  
Costa Mesa, CA 92627

Paul L. Richards  
Department of Physics  
University of California  
Berkeley, CA 94720

Arthur Robinson  
Science Magazine  
1515 Massachusetts Ave. N.W.  
Washington, DC 20005

Joel W. Russell  
Department of Chemistry  
Oakland University  
Rochester, MI 48063

Roger Ryberg  
Physics Department  
Chalmers University of Technology  
S-412 96 Gothenburg, SWEDEN

David Saperstein  
IBM A62/44  
San Jose, CA 95193

- Allen Sault**  
118 Mirrieles  
Stanford, CA 94305
- Roberta P. Saxon**  
SRI International  
333 Ravenswood Avenue  
Menlo Park, CA 94025
- Kerin Scanlon**  
Chemistry Department  
207 Pleasant SE  
University of Minnesota  
Minneapolis, MN 55455
- Juergen Schaefer**  
Physics Department  
Montana State University  
Bozeman, MT 59717
- George Schatz**  
Department of Chemistry  
Northwestern University  
Evanston, IL 60201
- Zack Schlesinger**  
Bell Laboratories  
600 Mountain Avenue  
Murray Hill, NJ 07974
- D. Schmeisser**  
Fritz-Haber Institut  
Faradayweg 4-6  
1000 Berlin - West  
WEST GERMANY
- K. Schoenhammer**  
I. Institut fuer  
Theoretical Physik  
Universitaet Hamburg  
D-2000 Hamburg  
WEST GERMANY
- Hajime Seki**  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193
- Gary Selwyn**  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193
- Mark Severson**  
Department of Chemistry  
University of Minnesota  
Minneapolis, MN 55455
- N. Sheppard**  
School of Chemical Sciences  
University  
Norwich, Norfolk NR4 7TJ  
ENGLAND
- Steven J. Sibener**  
James Franck Institute  
University of Chicago  
5640 S. Ellis Ave.  
Chicago, IL 60637
- David M. Silver**  
Johns Hopkins University  
Applied Physics Laboratory  
Laurel, MD 20707
- Paul Stevens**  
3353 Alma St., #139  
Palo Alto, CA 94306
- James P. Stone**  
Center for Laser Studies  
University of Southern California  
Los Angeles, CA 90082-1112
- Roger L. Strong**  
E203 Colorado Apts.  
Lake Austin Blvd.  
Austin, TX 78703
- Eric Stuve**  
Department of Chem. Eng.  
Stanford University  
Stanford, CA 94305
- Wataru Suetaka**  
Fac. Eng.  
Tohoku University  
Sendai, JAPAN
- Jerome D. Swalen**  
IBM Research Laboratory  
K32/281  
San Jose, CA 95193
- Noriko Tani**  
Department of Chemistry  
Kwansei Gakuin University  
Nishinomiya 662, JAPAN

C. G. Tengstal  
Department of Physics  
Chalmers University of Technology  
S-41296 Goteborg  
SWEDEN

Patricia Thiel  
Sandia National Laboratories  
Livermore, CA 94550

Paul A. Thiry  
F.N.D.P.  
61, rue de Bruxelles  
5000 Namur, BELGIUM

Roger G. Tobin  
Department of Physics  
University of California  
Berkeley, CA 94720

Brian Toby  
California Institute of Technology  
206-41  
Pasadena, CA 91125

Frank Trager  
IBM Research Laboratory  
K33/281  
San Jose, CA 95193

Hiromu Ueba  
Department of Electronics  
Toyama University  
Takaoka, Toyama, JAPAN

S. Ushioda  
Department of Physics  
University of California  
Irvine, CA 92717

R. Viswanathan  
Department of Chemistry  
Northwestern University  
Evanston, IL 60201

H. Weinberg  
California Institute of Technology  
206-41  
Pasadena, CA 91125

Eric Weitz  
Department of Chemistry  
Northwestern University  
Evanson, IL 60201

Eugene Wells  
Physical Review Letters  
Ridge, NY 11961

John F. Wendelken  
P. O. Box X, ORNL Bldg. 3025  
Oak Ridge, TN 37830

Charles Wong  
IBM Corp. 34A/006  
5600 Cottle Road  
San Jose, CA 95193

Haruka Yamada  
Department of Chemistry  
Kwansei Gakuin University  
Nishinomiya 662, JAPAN

Chien-fan Yu  
The James Franck Institute  
The University of Chicago  
5375 S. Ellis Ave.  
Chicago, IL 60637

**Vibrations at Surfaces**

**Proceedings of the Third International Conference,  
Asilomar, California, U.S.A., 1–4 September 1982**

**Part A**

Edited by

**C.R. BRUNICLE and H. MORAWITZ**

*IBM Research, 5600 Cottle Road, San José, CA 95193, U.S.A.*

8461057  
8461057  
Complete Contents of the Proceedings of the Third International Conference,  
Asilomar, California, U.S.A., 1-4 September 1982

TABLE OF CONTENTS

**Part A**

Contents of Volume 29 (the first of two Conference volumes)

Foreword .....	XV
List of Participants .....	XVII

LIST OF PAPERS PRESENTED  
(Invited papers marked by asterisk.)

Introductory Keynote

Hot Atoms and Cold Facts: Mysteries and Opportunities in Vibration-Assisted Surface Chemistry  
C.B. Duke,\* Xerox Webster Research Center, Rochester, New York . . . . . 1

Session I: Vibrational Frequency Shifts and Widths; Lateral Interactions

Phase and Bonding Transitions in Chemisorbed Layers Studied by Vibrational Frequency Shifts  
D.A. King,\* University of Liverpool, England . . . . . 11

Combined Vibrational/Temperature Programmed Reaction Spectroscopy Studies of Reaction Intermediates on Metal Surfaces  
R.J. Madix,\* Stanford University, Stanford, California . . . . . 25

High Resolution Infrared Study of Hydrogen Chemisorbed on Si(100)  
Y.J. Chabal, E.E. Chaban and S.B. Christman, Bell Laboratories, Murray Hill, New Jersey . . . . . 35

Thermal Scattering of Slow Electrons During Elastic Specular Reflection from a Cu(001) Surface  
R.E. Dietz, E.G. McRae and D.A. Kapilow, Bell Laboratories, Murray Hill, New Jersey . . . . . 41

Lateral Interactions and Vibrational Lifetimes  
B.N.J. Persson,\* KFA, Jülich, West Germany . . . . . 43

The Oxidation of Methanol on Cu(100) Studied by Infrared Spectroscopy  
R. Ryberg, Chalmers University of Technology, Sweden . . . . . 59

Vibrations Spectra of Oxygen Chemisorbed on Nickel(110) Surfaces  
G. Allan, Institut Supérieur d'Électronique du Nord, Lille Cedex, France and J. Lopez, Université Claude Bernard, Villeurbanne Cedex, France . . . . . 61

Dipole-Dipole Coupling in Adsorbate Vibrational Mode Spectra  
Z. Schlesinger, Bell Laboratories, Murray Hill, New Jersey, and A.J. Sievers, Cornell University, New York . . . . . 67

The Reflection-Absorption Infrared Spectrum of the Dioxygen Species Adsorbed on Platinum recorded by FT-IR Spectroscopy  
N.D.S. Canning and M.A. Chesters, University of East Anglia, Norwich, England . . . . . 69

Ab Initio CI Investigation of Hydrogen Atom Adsorption on Li Clusters: Embedded Cluster Model  
Hans-Ottmar Beckmann, State University of New York, New York . . . . . 77

Investigation of Lateral Interactions in Chemisorption  
Inder P. Batra, IBM Research Laboratory, San José, California . . . . . 83