FINAL REPORT

Office of Naval Research

Grant No. N00014-90-J-1581

for

Partial Funding of Gordon Research Conference

"Fundamental Interactions of Water with Solid Surfaces"

July 16-20, 1990

Kimball Union Academy

Meriden, NH

Submitted by:

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A. ORIGINATING AGENCY

Office of Naval Research

B. REPORT TITLE AND/OR NUMBER

Partial Funding of Gordon Research

C. MONITOR REPORT NUMBER

Gordon Research

D. PREPARED UNDER CONTRACT NUMBER

D00014-90-J-1581

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1990 Gordon Research Conference on
"Fundamental Interactions of Water with Solid Surfaces"

The Gordon Conference on the "Fundamental Interactions of Water with Solid Surfaces" was held from July 16 to 20, 1990 at the Kimball Union Academy in Meriden, NH. The Chairman was Theodore E. Madey of Rutgers University; the Vice-Chairperson was Patricia A. Thiel of Iowa State University. The conference attracted sixty participants; about twenty five percent were from foreign countries, including Canada. There was a good mixture of scientists from universities, national laboratories and private industries, including young scientists and graduate students as well as established scientists.

The program brought together people working in rather different areas, including surface chemistry and physics, electrochemistry, corrosion, wetting, fracture, and processing of semiconductors. The program included eighteen lecturers and nine discussion leaders. The discussion following the talks was unusually active and stimulating, and a large percentage of the attendees contributed to the discussion.

There were a number of exciting new results presented and discussed. P. Norton presented high sensitivity reflection infrared absorption spectroscopic measurements of H_2O on Ni(110), and correlated his results with absolute coverage determinations. Bonzel and White discussed the role of surface additive atoms on the structure and chemistry of H_2C, and demonstrated that a "critical coverage" of adsorbed alkali is necessary for H_2O dissociation to occur. Molecular dynamics simulations of H_2O on metal and oxide surfaces were well covered by Spohr and Garofalini, and their results provided new insights into the structure and reactivity of adsorbed H_2O. Stuve and Wagner described the linkage between surface science and electrochemistry in H_2O-solid interactions, and Wagner reported positive evidence for adsorbed hydronium, H_3O^+. Chabal described the use of aqueous HF for producing atomically smooth and clean Si(111) surfaces, and Sinclair described the problems caused by moisture in failure of semiconductor electronics.

The role of moisture in fracture of brittle materials was discussed by Lawn, and Porter presented exciting evidence for the structure of H_2O layers between two surfaces at distances of the order 1 nm. Dubois provided the first convincing data showing the relation between surface science (thermal desorption) measurements and macroscopic wetting of surfaces. Finally, Campbell and Kasemo described detailed kinetic schemes for the formation and decomposition of H_2O.
There were two poster sessions containing a total of twenty four posters of high calibre. All reports I received indicated that the conference was successful and stimulating. The next Gordon Conference on this subject will be scheduled in four to five years, under the chairmanship of Prof. Patricia Thiel, Iowa State University.

Attachments:
1. Conference Program
2. List of Poster Presentations
3. Attendance List
GORDON RESEARCH CONFERENCE

"Fundamental Interactions of Water With Solid Surfaces"
Kimball Union Academy, Meriden, New Hampshire

Theodore E. Madey, Chairman
Rutgers University

Patricia A. Thiel, Vice Chairman
Iowa State University

July 16-20, 1990

Sunday, July 15, 1990

7:00 p.m. Dinner
8:00 p.m. Mixer

Monday, July 16, 1990

8:45 a.m. Introductory Remarks

Morning Session: Water-Metal Interactions

Carsten Benndorf, Discussion Leader

9:00 a.m. Peter Norton
University of Western Ontario
"Interaction of Water with Nickel and Aluminum Surfaces: Absolute Coverages, Ordering and Dynamics"

9:50 a.m. Discussion

10:20 a.m. Coffee; Conference Photograph

10:40 a.m. Jose M. Heras
University Nacional de La Plata, Argentina
"Water on Polycrystalline Metal Surfaces"

11:30 a.m. Discussion

12:30 p.m. Lunch

Evening Session: Water Interactions With Additives

Galen B. Fisher, Discussion Leader

7:00 p.m. H. P. Bonzel
KFA Julich
"Alkali-Modified Adsorption of Water"

7:35 p.m. Discussion

8:00 p.m. J. M. White
University of Texas
"Surface Science of Coadsorbate Overlayers Involving Water"

8:35 p.m. Discussion
Tuesday, July 17, 1990

Morning Session: Theory of H₂O Layers on Surfaces

Uzi Landman, Discussion Leader

9:00 a.m. Eckhard Spohr
University of California
"Computer Simulations of Water on Metal Surfaces"

9:50 a.m. Discussion

10:25 a.m. Coffee

10:40 a.m. J. Woods Halley, Jr.
University of Minnesota
"Electronic Structure and Dynamics at the Water/Electrode Interface"

11:30 a.m. Discussion

12:30 p.m. Lunch

Evening Session: Water at Oxide Surfaces

Richard L. Kurtz, Discussion Leader

7:00 p.m. Victor E. Henrich
Yale University
"The Interaction of Water with Perfect and Defect Surfaces of Semiconductors and Oxides"

7:35 p.m. Discussion

7:50 p.m. Stephen H. Garofalini
Rutgers University
"Water Interactions with Oxide Glass Surfaces - Molecular Dynamics Simulations"

8:25 p.m. Discussion

8:40 p.m. Poster Session

Wednesday, July 18, 1990

Morning Session: Electrochemical Aspects of Water-Surface Interactions

P. N. Ross, Jr., Discussion Leader

9:00 a.m. Eric Stuve
University of Washington
"In-Situ and Ex-Situ Studies of Electrochemical Phenomena"

9:50 a.m. Discussion

10:25 a.m. Coffee

10:40 a.m. Frederick T. Wagner
General Motors Research Labs
"UHV Investigations of Surface Solvation Effects in Electrochemistry"

11:30 a.m. Discussion

12:30 a.m. Lunch
Evening Session: Interaction of Water With Electronic Materials

Patricia M. George, Discussion Leader

7:00 p.m. Yves Chabal
AT&T Bell Laboratories
"Infrared Spectroscopy of Water - Modified Silicon Surfaces"

7:35 p.m. Discussion

7:50 p.m. J. D. Sinclair
AT&T Bell Laboratories
"The Role of Water in the Degradation of Electronics: Materials, Mechanisms, Protection, and Challenges"

8:25 p.m. Discussion

8:40 p.m. Poster Session

Thursday, July 19, 1990

Morning Session: Interfacial Phenomena

Bruce Bunker, Discussion Leader

9:00 a.m. Brian Lawn
National Institute of Standards and Technology
"Surface Forces, Adhesion and Fracture of Brittle Solids"

9:50 a.m. Discussion

10:25 a.m. Coffee

10:40 a.m. John D. Porter
Univ. of California, Berkeley
"Interfacial Structure and Dynamics in Hg/H2O/Hg Tunnel Junction Devices"

11:30 a.m. Discussion

12:30 p.m. Lunch

Evening Session: Wetting Phenomena

Mark O. Robbins, Discussion Leader

7:00 p.m. Michael Schick
University of Washington
"A Theoretical Overview of Wetting Phenomena"

7:35 p.m. Discussion

8:00 p.m. Lawrence H. Dubois
AT&T Bell Laboratories
"Wetting of Organic Surfaces: Microscopic Predictions of a Macroscopic Observable"

8:35 p.m. Discussion
Friday, July 20, 1990

Morning Session: Reactions of H₂O at Surfaces

John T. Yates, Jr., Discussion Leader

8:45 a.m. Charles T. Campbell
University of Washington

9:35 a.m. Discussion

10:00 a.m. Coffee

10:15 a.m. Bengt Kasemo
Chalmers Univ. of Technology
“Water Formation and Decomposition on Pt”

11:05 a.m. Discussion

12:00 noon Lunch
Posters Presented at Gordon Conference

"Fundamental Interactions of Water with Solid Surfaces"

Tuesday, July 17, 1990

Dr. G. Pirug
Institut für Grenzflächenforschung
Forschungszentrum Jülich GmbH
Postfach 1913
D-51170 Jülich 1
Federal Republic of Germany

"The Influence of Alkali Metals on the Oxidation of Si(100) Surfaces by H2O"
(Authors: G. Pirug and H. P. Bonzel)

Dr. A. Brodsky
Department of Chemistry
University of Pennsylvania
Philadelphia, PA 19104-6323

"Phase Transitions in Surface Water Layers"

Professor Jiri Skvarla
Department of Mineral Processing and Environmental Protection
Technical University
Park Komenskeho 19
043 84 Kosice
Czechoslovakia

"A Correlation Between the Wettability and Aggregation of Fine Minerals"

Robert Brosseau
Department of Chemistry
University of Montreal
Montreal, Quebec, CANADA

"Water on Pd(110)"
(Authors: R. Brosseau and T. H. Ellis)

Brian W. Callen
Department of Chemistry
University of Western Ontario
CANADA N6A 5B7

"Identification of Surface Water Molecules on Isotopically Substituted Ice Layers"
(Authors: Brian W. Callen, K. Griffiths and P. R. Norton)

Professor J. A. Panitz
Department of Physics and Astronomy
The University of New Mexico
Albuquerque, NM 87131

"Imaging Atom-Probe Studies of Aqueous Interfaces"

Eric K. Parks
Argonne National Laboratory
701 Lakeside Drive
Hinsdale, IL 60521

"Reactions of Water with Iron, Cobalt, and Nickel Clusters"
(Authors: E. K. Parks, S. Riley, T. Klots and B. Winter)
Stephen James Bushby
Department of Chemistry
University of Western Ontario
London, Ontario
CANADA N6A 5B7

"Absolute Hydroxyl Coverage of Oxides Formed by Water Interaction with Al(100)"

Si-Chung Chang
Department of Chemistry
Purdue University
West Lafayette, IN 47907-3699

"In-Situ Infrared Spectroscopy of Well-Defined Single Crystal Electrodes"
(Authors: S.-C. Chang and M. Weaver)

Yitzhak Shnidman
Research Laboratories
Eastman Kodak Company
Rochester, NY 14650-2109

"Concentration-Driven Surface Transition in the Wetting of Mixed Alkanethiol Monolayers"
(Authors: Y. Shnidman, J. E. Eilers, S. D. Evans, R. Sharma, J. C. Chang and A. Ulman)

W.-H. Hung
Department of Chemistry
Princeton University
Princeton, NJ 08544

"The Adsorption of H_2O on Clean and Oxidized Fe(100)"
(Authors: W.-H. Hung, J. Schwartz and S. L. Bernasek)

Wednesday, July 18, 1990

Dr. Geoff Thornton
Chemistry Department
Manchester University
Manchester M13 9PL
United Kingdom

"H_2O Adsorption on BSSCO (001) and Other Oxide Surfaces"

Dr. Rudolf Schubert
Room 3X 215
Bellcore
P. O. Box 7040
Red Bank, NJ 07701-7040

"The Effect of Relative Humidity on Electrical Contacts"

Dr. Richard Kurtz
Surface Science Division
National Institute for Science and Technology
Gaithersburg, MD 20899

"The Role of Surface Defects in Water Chemisorption on TiO_2(110)"
Dr. Ben Ocko  
Department of Physics  
Brookhaven National Laboratory  
Upton, Long Island, NY 11973

"In-Situ X-ray Scattering Investigations of Electrode Surface Reconstructions"

Dr. Brian Maschhoff  
Department of Physics  
Laboratory for Surface Modification  
Rutgers, The State University of New Jersey  
P. O. Box 849  
Piscataway, NJ 08855-90849

"Interaction of Water with Insulator Surfaces"  
(Authors: Brian Maschhoff, J. M. Pan, M. Szymonski and T. E. Madey)

Dr. D. R. Baer  
Surface Physics Group  
Battelle Pacific NW Lab  
Battelle Blvd.  
Richland, WA 99352

"Interactions of H₂O and Mn with the Cleavage Surface of CaCO₃"  
(Authors: D. R. Baer, D. L. Blanchard and J. M. Zachara)

Prof. Andrej Wieckowski  
Department of Chemistry  
University of Illinois  
Urbana, IL 61801

"Voltammetry and Surface Science of Rh(100) and Rh(111) Surfaces"

Dr. Masakatsu Watanabe  
Department of Chemistry  
University of Pennsylvania  
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"Phase Transition of Water Between Metal Surfaces"

Dr. Fred Wagner  
Physical Chemical Dept.  
General Motors Research Labs  
30500 Mound Road  
Warren, MI 48090-9055

"Hydrogen and Water Coadsorption on Cu(110) and Pt(111): the Formation of H₃O⁺?"

Prof. J. Michael White  
Department of Chemistry  
University of Texas  
Austin, Texas 78712

"Optical Absorption of H₂O(g) and Amorphous Ice"

Dr. Patricia M. George  
Aerojet Electro Systems  
Surface and Contam. Dept.  
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"The Reaction of Water on GaAs(100)"
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"An XPS Study of Water Removal from Be at 160K: Evidence for Ion Beam-Induced Oxidation"

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Department of Chemistry  
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"Molecular Diffusion on Solid Surfaces: How Chemisorbed Molecules Differ from Atoms"
GORDON RESEARCH CONFERENCES

FUNDAMENTAL INTERACTION OF WATER WITH SOLID SURFACES

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July 16 - 20, 1990

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