

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

**2002 GORDON RESEARCH CONFERENCE
on WATER & AQUEOUS SOLUTIONS
FINAL PROGRESS REPORT**

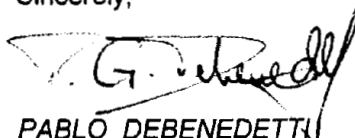
DEPARTMENT OF ENERGY
GRANT NO. DE-FG02-02ER15310

The Gordon Research Conference (GRC) on WATER & AQUEOUS SOLUTIONS was held at Holderness School from 8/4/02 thru 8/9/02. The Conference was well-attended with 123 participants (attendees list attached). The attendees represented the spectrum of endeavor in this field coming from academia, industry, and government laboratories, both U.S. and foreign scientists, senior researchers, young investigators, and students.

In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field. There was a conscious effort to stimulate lively discussion about the key issues in the field today. Time for formal presentations was limited in the interest of group discussions. In order that more scientists could communicate their most recent results, poster presentation time was scheduled. Attached is a copy of the formal schedule and speaker program and the poster program. In addition to these formal interactions, "free time" was scheduled to allow informal discussions. Such discussions are fostering new collaborations and joint efforts in the field.

I want to personally thank you for your support of this Conference. As you know, in the interest of promoting the presentation of unpublished and frontier-breaking research, Gordon Research Conferences does not permit publication of meeting proceedings. If you wish any further details, please feel free to contact me. Thank you.

Sincerely,



PABLO DEBENEDETTI
PRINCETON UNIVERSITY

WATER & AQUEOUS SOLUTIONS

August 4-9, 2002
Holderness School
Plymouth, NH

Chairs: **Pablo Debenedetti & John Finney**
Vice-Chairs: **Alfons Geiger & Richard Saykally**

SUNDAY

2:00 pm - 9:00 pm Arrival and check-in

5:00 pm - 6:00 pm Chair's reception

6:00 pm Dinner

7:30 pm - 9:30 pm **WET EARTH - HOW OUR PLANET WORKS**

[[click here for detailed session information](#)]

Discussion Leader: **Alan Thompson** (ETH-Zürich, Switzerland)

7:30 pm - 7:40 pm **Alan Thompson** (ETH-Zürich, Switzerland)
Introductory remarks

7:40 pm - 8:35 pm **Greg Hirth** (Woods Hole Oceanographic Institute, USA)
"Why water is required for the unique plate-like behavior of the Earth"

8:35 pm - 9:30 pm **Craig Manning** (University of California, Los Angeles, USA)
"In deep water: dense aqueous solutions and their role in Earth's evolution"

MONDAY

7:45 am - 8:45 am Breakfast

8:45 am Conference photo

9:00 am - 12:30 am **WATER IN AEROSOLS AND CLOUDS**

[[click here for detailed session information](#)]

Discussion Leader: **Thomas Peter** (ETH-Zürich, Switzerland)

9:00 am - 9:15 am **Thomas Peter** (ETH-Zürich, Switzerland)
Introductory remarks

9:15 am - 10:10 am **Marcia Baker** (University of Washington, Seattle, USA)
"The roles of water in cloud radiative and electrical phenomena"

10:10 am - 10:40 am Coffee break

10:40 am - 11:35 am **Thomas Koop** (ETH-Zürich, Switzerland)
"Metastable aqueous solutions in atmospheric aerosol droplets"

11:35 am - 12:30 pm **Maria Cristina Facchini** (Inst. Atmosph. & Climate Sci., Italy)
"Chemical effects on cloud activation with special emphasis on the effect of organic compounds"

12:30 pm Lunch

4:00 pm - 6:00 pm Poster session

6:00 pm Dinner

7:30 pm - 9:30 pm **AMORPHOUS, SUPERCOOLED AND GLASSY WATER**

[[click here for detailed session information](#)]

Discussion Leader: **Erwin Mayer** (University of Innsbruck, Austria)

7:30 pm - 7:40 pm **Erwin Mayer** (University of Innsbruck, Austria)
Introductory remarks

7:40 pm - 8:35 pm **Alan Soper** (Rutherford Laboratory, Chilton, UK)

- 8:35 pm - 9:30 pm **The structure of the low temperature forms of water as seen by neutron diffraction"**
C. Austen Angell (Arizona State University, Tempe, USA)
 "Exploring water in "No-Man's Land" by parallel annealing studies of hyperquenched samples of water and solutions"

TUESDAY

7:45 am - 8:45 am Breakfast

9:00 am - 12:30 am **AQUEOUS SOLUTIONS**[[click here for detailed session information](#)]Discussion Leader: **Ed Castner** (Rutgers University, USA)9:00 am - 9:15 am **Ed Castner** (Rutgers University, USA)
Introductory remarks9:15 am - 10:10 am **Daniel Bowron** (Rutherford Laboratory, Chilton, UK)
"Ion-amphiphile interactions in aqueous solution"

10:10 am - 10:40 am Coffee break

10:40 am - 11:35 am **Kenneth Harris** (Australian Defence Force Academy, Australia)
"Molecular motion and solution structure: high pressure diffusion studies of water and aqueous solutions of amphiphilic solutes"11:35 am - 12:30 pm **Giulia Galli** (Lawrence Livermore National Laboratory, USA)
"Ab-initio simulations of water under pressure and of simple aqueous solutions"

12:30 pm Lunch

4:00 pm - 6:00 pm Poster session

6:00 pm Dinner

7:30 pm - 9:30 pm **BIOPRESERVATION AND PHYSICAL CHEMISTRY IN LOW-MOISTURE FORMULATIONS**[[click here for detailed session information](#)]Discussion Leader: **Christopher Roberts** (Pfizer, Groton, USA)7:30 pm - 7:40 pm **Christopher Roberts** (Pfizer, Groton, USA)
Introductory remarks7:40 pm - 8:20 pm **George Zograf** (University of Wisconsin, Madison, USA)
"Factors influencing water vapor absorption by amorphous solids at various relative humidities"8:20 pm - 8:55 pm **Michael Pikal** (University of Connecticut, Storrs, USA)
"The effect of water on the physical and chemical properties of proteins in the solid state: protein structure, dynamics, and pharmaceutical stability"8:55 pm - 9:30 pm **Juan dePablo** (University of Wisconsin, Madison, USA)
"Cryoprotectants and lyoprotectants in solution. Structure, properties, and their relation to biopreservation efficacy"**WEDNESDAY**

7:45 am - 8:45 am Breakfast

9:00 am - 12:30 am **SELF-ASSEMBLY IN WATER**[[click here for detailed session information](#)]Discussion Leader: **Adrian Parsegian** (National Institutes of Health, USA)9:00 am - 9:15 am **Adrian Parsegian** (National Institutes of Health, USA)
Introductory remarks9:15 am - 10:10 am **Robert Prud'homme** (Princeton University, USA)
"Polysaccharide association in aqueous solution"

10:10 am - 10:40 am Coffee break

10:40 am - 11:35 am **Sergey Leikin** (National Institutes of Health, USA)
"How nature uses the properties of water to organize the protein matrix of skin and bone"11:35 am - 12:30 pm **John Nagle** (Carnegie-Mellon University, Pittsburgh, USA)
"Structure and interactions in fully hydrated lipid bilayers determined using new diffuse x-ray diffraction methods"

12:30 pm Lunch
 4:00 pm - 6:00 pm Poster session
 6:00 pm Dinner
 7:30 pm - 9:30 pm **STRUCTURE AND DISSOCIATION DYNAMICS IN TETRAHEDRAL LIQUIDS**

[[click here for detailed session information](#)]

Discussion Leader: **Frank Stillinger** (Princeton University, USA)

7:30 pm - 7:40 pm **Frank Stillinger** (Princeton University, USA)
 Introductory remarks

7:40 pm - 8:35 pm **Francesco Sciortino** (University of Rome, Italy)
 "Potential energy landscape in water and silica. Basins and saddles"

8:35 pm - 9:30 pm **Christoph Dellago** (University of Rochester, USA)
 "Proton conduction through water-filled carbon nanotubes"

THURSDAY

7:45 am - 8:45 am Breakfast

9:00 am - 12:30 am **WATER IN EXTREME BIOLOGICAL SYSTEMS**

[[click here for detailed session information](#)]

Discussion Leader: **Roy Daniel** (University of Waikato, New Zealand)

9:00 am - 9:15 am **Roy Daniel** (University of Waikato, New Zealand)
 Introductory remarks

9:15 am - 10:10 am **Peter Halling** (University of Strathclyde, Glasgow, UK)
 "Enzyme action in (relatively) low water media"

10:10 am - 10:40 am Coffee break

10:40 am - 11:35 am **C. Nick Pace** (Texas A&M University, USA)
 "How water affects protein stability"

11:35 am - 12:30 pm **William McKinnon** (Washington University, USA)
 "Water on Europa"

12:30 pm Lunch

4:00 pm - 6:00 pm Poster session

6:00 pm Banquet

7:30 pm - 8:00 pm Business meeting, elections, etc.

8:00 pm - 9:00 pm **THIRTY YEARS AFTER RAHMAN AND STILLINGER'S FIRST SIMULATION: WHAT HAVE WE LEARNED AND WHAT MIGHT COME NEXT?**

[[click here for detailed session information](#)]

Discussion Leader: **Alfons Geiger** (University of Dortmund, Germany)

8:00 pm - 9:00 pm **David Chandler** (University of California, Berkeley, USA)
 "Thirty years after Rahman and Stillinger's first simulation: what have we learned and what might come next?"



WATER & AQUEOUS SOLUTIONS

Holderness School
Aug 4-9, 2002

NOTE: Receipt of Application does not guarantee acceptance to a Conference. Applications are reviewed by the Conference Chair. If the Chair approves your application, you become **Accepted** and you will be sent a personalized link to the GRC online registration site. When you complete the online registration, you become **Registered**.

Only those who have been **Accepted** or **Registered** will have their names listed below. Names of people who have only applied and have yet to be accepted will NOT appear.

Name	Organization	Participation	Status
C. AUSTEN ANGELL	ARIZONA STATE UNIVERSITY	Speaker	Registered
DAVID J ANICK	HARVARD MEDICAL SCHOOL	Poster Presenter	Registered
HANK ASHBAUGH	LOS ALAMOS NATIONAL LABS	Poster Presenter	Registered
ADEBAYO G AUGUSTINE	UNIVERSITY OF AGRICULTURE, ABEOKUTA	Poster Presenter	Registered
MARCIA BAKER	UNIVERSITY OF WASHINGTON	Speaker	Registered
MARIE-CLAIRE BELLISSENT-FUNEL	LABORATOIRE LÉON BRILLOUIN (CEA-CNRS)	Poster Presenter	Registered
ALBERTO BOTTI	UNIVERSITY OF ROMA TRE	Poster Presenter	Registered
DANIEL T BOWRON	ISIS FACILITY	Speaker	Registered
FABIO BRUNI	UNIVERSITA DI ROMA TRE	Poster Presenter	Registered
VICTORIA BUCH	THE HEBREW UNIVERSITY	Poster Presenter	Registered
PIERS BUCHANAN	KING COLLEGE LONDON	Attendee	Registered
SERGEY V BULDYREV	BOSTON UNIVERSITY	Poster Presenter	Registered
BERNARD F CABANE	CNRS	Attendee	Registered
EDWARD W CASTNER	RUTGERS UNIVERSITY	Discussion Leader	Registered
DAVID CHANDLER	UNIVERSITY OF CALIFORNIA, BERKELEY	Speaker	Registered
MARTIN F CHAPLIN	SOUTH BANK UNIVERSITY	Poster Presenter	Registered
YNG-GWEI CHEN	UNIVERSITY OF MARYLAND	Poster Presenter	Registered
VIORÉL C CHIHAIA	MINERAL.-KRISTALLOGR. INSTITUT DER UNIVERSITÄT GÖ	Poster Presenter	Registered
JASON CRAIN	UNIVERSITY OF EDINBURGH	Attendee	Registered
ROY M DANIEL	UNIVERSITY OF WAIKATO	Discussion Leader	Registered
FRANCOIS H DAVID	CNRS	Poster Presenter	Registered
JUAN J DE PABLO	UNIVERSITY OF WISCONSIN, MADISON	Speaker	Registered
PABLO DEBENEDETTI	PRINCETON UNIVERSITY	Chair	Registered
CHRISTOPH DELLAGO	UNIVERSITY OF ROCHESTER	Speaker	Registered
ALFRED DELVILLE	CNRS-CRMD	Poster Presenter	Registered
J. PAUL DEVLIN	OKLAHOMA STATE UNIVERSITY	Monitor	Registered
SOFIA DIAZ MORENO	ESRF	Attendee	Registered
RALPH C DOUGHERTY	FLORIDA STATE UNIVERSITY	Poster Presenter	Registered
RACHEL V DUNN	UNIVERSITY OF WAIKATO	Attendee	Registered
CHARLES D EADS	P&G CORPORATE RESEARCH DIVISION	Poster Presenter	Registered
JOEL D EAVES	MASSACHUSETTS INSTITUTE OF TECHNOLOGY	Poster Presenter	Registered
JEFFREY R ERRINGTON	UNIVERSITY AT BUFFALO	Poster Presenter	Registered
MARIA CRISTINA FACCHINI	INSTITUTE OF ATMOSPHERIC & CLIMATE SCIENCES (ISAC)	Speaker	Registered
MELISSA R FEENEY	PRINCETON UNIVERSITY	Poster Presenter	Registered
JOHN L FINNEY	UNIVERSITY COLLEGE LONDON	Chair	Registered
GIULIA GALLI	LAWRENCE LIVERMORE NATIONAL LABORATORY	Speaker	Registered
SHEKHAR S GARDE	RENSSELAER POLYTECHNIC INSTITUTE	Poster Presenter	Registered
ANA M GASPAR	CENTRO DE FISICA DA MATERIA CONDENSADA DA UL	Poster Presenter	Registered
ALFONS GEIGER	UNIVERSITAET DORTMUND	Vice Chair	Registered
BURKHARD GEIL	TECHNISCHE UNIVERSITAET DARMSTADT	Attendee	Registered
PHILLIP L GEISSLER	M.I.T.	Attendee	Registered
HAGGAI GILBOA	TECHNION - IIT	Attendee	Registered

NICOLAS GIOVAMBATTISTA	BOSTON UNIVERSITY	Poster Presenter	Registered
NIR GOLDMAN	UNIVERSITY OF CALIFORNIA BERKELEY	Poster Presenter	Registered
NIKOLAY V GOUTEV	CREST, JAPAN SCIENCE AND TECHNOLOGY CORPORATION	Poster Presenter	Registered
ANDREAS HALLBRUCKER	UNIVERSITY OF INNSBRUCK	Attendee	Registered
PETER HALLING	UNIVERSITY OF STRATHCLYDE	Speaker	Registered
MICHAEL R HARPHAM	COLORADO STATE UNIVERSITY	Poster Presenter	Registered
KENNETH R HARRIS	UNIVERSITY COLLEGE (UNSW)	Speaker	Registered
MICHAEL B HAY	PRINCETON UNIVERSITY	Poster Presenter	Registered
BALAZS HETENYI	PRINCETON UNIVERSITY	Poster Presenter	Registered
GREG HIRTH	WOODS HOLE OCEANOGRAPHIC INSTITUTION	Speaker	Registered
GREGORY L HURA	U.C. BERKELEY	Attendee	Registered
K. RUTH INESON	RETIRED	Attendee	Registered
HITOSHI KANNO	NATIONAL DEFENSE ACADEMY	Poster Presenter	Registered
BRUCE D KAY	PACIFIC NORTHWEST NATIONAL LABORATORY	Poster Presenter	Registered
CAROLYN A KOH	KING'S COLLEGE LONDON	Poster Presenter	Registered
INGRID KOHL	MASSACHUSETTS INSTITUTE OF TECHNOLOGY	Poster Presenter	Registered
THOMAS KOOP	SWISS FEDERAL INSTITUTE OF TECHNOLOGY	Speaker	Registered
PETER G KUSALIK	DALHOUSIE UNIVERSITY	Poster Presenter	Registered
ZDRAVKO KUTNJAK	JOZEF STEFAN INSTITUTE	Poster Presenter	Registered
BRANKA M LADANYI	COLORADO STATE UNIVERSITY	Monitor	Registered
ROBERT LAENEN	TU MUENCHEN, PHYSIK-DEPARTMENT E 11	Poster Presenter	Registered
JAEHO LEE	BROWN UNIVERSITY	Poster Presenter	Registered
SAU L LEE	PRINCETON UNIVERSITY	Attendee	Registered
SERGEY LEIKIN	NATIONAL INSTITUTES OF HEALTH	Speaker	Registered
CARRIE S LOCK	PRINCETON UNIVERSITY	Attendee	Registered
THOMAS LOERTING	MASSACHUSETTS INSTITUTE OF TECHNOLOGY	Poster Presenter	Registered
ALENKA LUZAR	UNIVERSITY OF CALIFORNIA SAN FRANCISCO	Poster Presenter	Registered
JALEL M'HALLA	FACULTÉ DES SCIENCES DE MONASTIR	Poster Presenter	Registered
CRAIG MANNING	UNIVERSITY OF CALIFORNIA, LOS ANGELES	Speaker	Registered
ABRAHAM MARMUR	TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY	Poster Presenter	Registered
DE BARROS M.I. MARQUES	C.FISICA MATERIA CONDENSADA UNIV. LISBOA	Poster Presenter	Registered
M. ALVES MARQUES	C. FIS. MAT. CONDENSADA	Poster Presenter	Registered
GLENN J. MARTYNA	IBM RESEARCH : PHYSICAL SCIENCES DIVISION	Poster Presenter	Registered
ERWIN MAYER	UNIVERSITAET INNSBRUCK	Discussion Leader	Registered
WILLIAM B MCKINNON	WASHINGTON UNIVERSITY	Speaker	Registered
JOSE ANTONIO MEJIAS	UNIVERSIDAD PABLO DE OLAVIDE	Poster Presenter	Registered
AKIHIRO MORITA	KYOTO UNIVERSITY	Poster Presenter	Registered
SATISH MYNENI	PRINCETON UNIVERSITY	Poster Presenter	Registered
JOHN F NAGLE	CARNEGIE MELLON UNIVERSITY	Speaker	Registered
THOMAS F O'CONNOR	PRINCETON UNIVERSITY	Attendee	Registered
CECILIA OLIVA	UNIVERSITA ROMA TRE	Poster Presenter	Registered
C N PACE	TEXAS A&M UNIVERSITY	Speaker	Registered
THOMAS PETER	INSTITUTE OF ATMOSHERIC AND ELIMATE SCIENCE	Discussion Leader	Registered
MICHAEL PIKAL	UNIVERSITY OF CONNECTICUT	Speaker	Registered
LAWRENCE PRATT	LOS ALAMOS NATIONAL LABORATORY	Attendee	Registered
ROBERT K PRUD'HOMME	PRINCETON UNIVERSITY	Speaker	Registered
ELIZABETH A RAYMOND	UNIVERSITY OF OREGON	Poster Presenter	Registered
GLEN REIN	ESTEE LAUDER COMPANIES	Attendee	Registered
MARIA A RICCI	UNIVERSITA' DEGLI STUDI ROMA TRE	Poster Presenter	Registered
CHRISTOPHER J ROBERTS	UNIVERSITY OF DELAWARE	Discussion Leader	Registered
YAROSLAV E RYABOV	THE HEBREW UNIVERSITY OF JERUSALEM	Poster Presenter	Registered
CHRISTOPH G SALZMANN	UNIVERSITY OF INNSBRUCK, AUSTRIA	Poster Presenter	Registered
RICHARD J SAYKALLY	UNIVERSITY OF CALIFORNIA, BERKELEY	Vice Chair	Registered
FRANCESCO SCIORTINO	UNIVERSITY OF ROME, LA SAPIENZA	Speaker	Registered
M. SCOTT SHELL	PRINCETON UNIVERSITY	Attendee	Registered
DAVID P SHELTON	UNIVERSITY OF NEVADA, LAS VEGAS	Poster Presenter	Registered
VINCENT SHEN	PRINCETON UNIVERSITY	Attendee	Registered
MUNIR S SKAF	STATE UNIVERSITY OF CAMPINAS	Poster Presenter	Registered
ANNA SKIBINSKY	BOSTON UNIVERSITY	Poster Presenter	Registered
NEIL SNIDER	NORTHWESTERN UNIVERSITY	Attendee	Registered
ALAN K SOPER	RUTHERFORD APPLETON LABORATORY	Speaker	Registered
FRANK H STILLINGER	PRINCETON UNIVERSITY	Discussion Leader	Registered
BERND STRUTH	ESRF	Poster Presenter	Registered

MICHAEL J TAUBER	UNIVERSITY OF CALIFORNIA BERKELEY	Poster Presenter	Registered
ALAN THOMPSON	INSTITUTE OF MINERALOGY & PETROGRAPHY	Discussion Leader	Registered
ANDREI TOKMAKOFF	MIT	Attendee	Registered
TOSHIHIRO TOMINAGA	OKAYAMA UNIVERSITY OF SCIENCE	Poster Presenter	Registered
THOMAS M TRUSKETT	UNIVERSITY OF TEXAS AT AUSTIN	Poster Presenter	Registered
PIERRE E TURQ	UNIVERSITE PIERRE ET MARIE CURIE	Poster Presenter	Registered
JACOB URQUIDI	ARGONNE NATIONAL LABS	Poster Presenter	Registered
GEORGE E WALRAFEN	UNIVERSITY OF KANSAS	Attendee	Registered
ROBIN E WESTACOTT	HERIOT-WATT UNIVERSITY	Poster Presenter	Registered
JUDITH WOLK	UNIVERSITAT ZU KÖLN	Poster Presenter	Registered
BARBARA E WYSLOUZIL	WORCESTER POLYTECHNIC INSTITUTE	Poster Presenter	Registered
YANFENG ZHANG	PRINCETON UNIVERSITY	Attendee	Registered
GEORGE D ZOGRFI	UNIVERSITY OF WISCONSIN, MADISON	Speaker	Registered

