

Standing Committees for

- Life, Earth and Environmental Sciences (LESC)
- Physical and Engineering Sciences (PESC)

SCIENTIFIC REPORT

ESF Exploratory Workshop on

EUROICE2008

Granada (Spain), 1-4 October 2008

Convened by:

C. Ignacio Sainz-Diaz and Julyan Cartwright

Instituto Andaluz de Ciencias de la Tierra (IACT), CSIC- Universidad de Granada, Spain

Co-sponsored by



Convenors:

C. Ignacio Sainz-Díaz

e-mail: cisainz@ugr.es

Laboratorio de Estudios Cristalográficos
Instituto Andaluz de Ciencias de la Tierra (IACT)
CSIC- Universidad de Granada
Edificio Instituto López Neyra
Av. del Conocimiento s/n
Parque Tecnológico de Ciencias de la Salud
18100-Armilla
Granada, Spain
Tel. 34-958-181644, Fax: 34-958-181632

Julyan Cartwright

e-mail: julyan@lec.csic.es

Instituto Andaluz de Ciencias de la Tierra, CSIC
Universidad de Granada
Av. Fuentenueva s/n
18002-Granada, Spain
Tel. 34-958-181644, Fax: 34-958-181632

Executive Summary

The scientific focus of this exploratory workshop was frontier research on ices from many experimental and theoretical points of view, including water ice and other ices or solids condensed from different gases existing in extreme conditions in space, polymorphism and polyamorphism of ice, nucleation, morphology, reactivity, spectroscopy, etc. There was a four-fold motivation:

- To identify the most pressing issues in the area of ices.
- For experimentalists in this area to compare the information content of different trials and techniques, and to develop multi-technique approaches to answer specific problems.
- For theoreticians and those working on computer simulations in this area to begin a work programme to exchange experience of different strategies and methodologies, to develop the optimum means of working, and to identify necessary developments in methodology and software.
- To develop a closer collaboration between experimentalists and theoreticians in the study of ices, in particular for experimentalists to define the information that needs to be provided by the theoreticians and vice versa.

The meeting fulfilled these aims extremely well; there were very good, thought-provoking talks from the participants. There were many interesting discussions between the participants after the talks, and also more informally in the breaks and in during the meals. The participants ate together at a large table in the meeting venue and this worked well as a means for facilitating the communication between participants. The same is true for the conference dinner and for the excursion to see the nearby Alhambra palace, where a guide specialist in symmetry groups showed some of the examples present in the monument.

It was anticipated that there should be a number of positive outcomes from the proposed workshop: the establishment of informal multi-approach collaborations and the definition of future EU-wide formal collaboration. One of the aims of this international meeting was to generate ideas for a future European network around these topics, related to the frontier researches on ices from different experimental and theoretical points of view, including a possible application for a funded EU network.

As planned, a number of informal collaborations has emerged from the workshop. Beyond that, the participants are engaged in writing a joint paper to review the field and to put forward the open questions that need to be addressed by the communities involved in ice research. The question of a formal collaboration based on applying for an EU or ESF funded network is currently being considered by the participants.

Scientific Report

As the workshop was designed to explore themes of ices, crystal growth, morphology, and interplanetary ices, the meeting was divided into sessions focusing on different themes within its remit:

Morphology and crystal growth of ices.

Julyan Cartwright (IACT, CSIC-UGR, Granada, Spain) described his joint work with Ignacio Sainz-Diaz on the morphology of ices in extreme conditions using the technique of ice growth in situ in a cryo-ESEM microscope. Applying the model of Zone Structures, the morphology of thin films of ice was discussed. Biomimetic forms of ice were obtained at extreme conditions of low temperature and pressure.

Debbie Stokes (FEI Instruments, UK) gave an overview of microscopy techniques of interest to those involved in research with ice, and showed results of her own and others' research. The new recent techniques of electron microscopy were presented.

Jan Pettersson (University of Goteborg, Sweden) discussed ice in the upper troposphere, including microphysics and climate effects, and presented the results of his research group in Gothenburg.

Jari Haapala (Finnish Institute of Marine Research, Helsinki, Finland) talked on geophysical models of sea-ice for the numerical investigations of climate based mainly on the Arctic region.

Vance Bergeron (ENS, Lyon, France) presented his work on penitentes: a typical morphology of the surface of glacial ice exposed to sunlight. A hot discussion was generated about the morphology of these ice-penitentes and some theoretical modeling works were presented.

Surface interactions with ices.

Davide Donadio (University of California in Davis, USA) gave a talk on IR and Raman spectroscopy of Ice from ab initio molecular dynamics and different crystal surfaces of silicon.

Emilio Artacho (Dept. of Earth Sciences, University of Cambridge, UK) discussed modelling of ice and water structures, including discrepancies on the hydrogen bond network of different polymorphs of ice.

Alfonso Hernández-Laguna (EEZ, CSIC, Granada, Spain) talked on the interaction of Ice on phyllosilicate surfaces by quantum mechanical calculations. A discussion was opened about the ordering of the first sheet of water molecules adsorbed on the silicate surfaces.

Stratospheric ices.

Hinrich Grothe (University of Vienna, Austria) discussed inter- and intra-molecular interactions in vibrations of nitric acid hydrates and vibrational IR spectra and X-ray diffraction studies of these samples.

Rafael Escribano (IEM, CSIC, Madrid, Spain) presented his group's results on laboratory study of ices related with stratospheric clouds and with cometary relevance: $\text{H}_2\text{O}/\text{CO}_2$, $\text{CO}_2/\text{HCH}_3\text{O}$; highlighting IR spectroscopy studies and theoretical calculations.

Nevin Uras-Aytemiz (Suleyman Demirel University, Turkey) discussed solid state solvation and ionization of HNO_3 on/in water clusters and ice and presented results based on dynamics and infrared spectroscopy.

Physics of ices.

Oreste Piro (Universidad de las Islas baleares, Mallorca) asked the question 'Is there an HDA-LDA transition in 2D?' and presented preliminary results of simulations with a non-linear physical model related with the surface morphology of vapor deposition.

Ray Goldstein (DAMPT, University of Cambridge, UK) presented his research into the shapes of icicles in the crystal growth and during melting.

John Finney (University College London, London, UK) talked on order and disorder in ice structures, discussing the limits between the different polymorphs and polyamorphs of ice.

Astrophysics and ices.

Gianni Strazzulla (Sicilia ,Italy) presented an overview of physico-chemical properties of astrophysical ices, and the research being carried out by his group in Sicily, related with the ion bombardment and derivate chemical and spectroscopy properties

Pedro Gutiérrez (IAA, CSIC, Granada) described work on macroscopic thermophysical modelling of thin layers of amorphous water ice wih applications to cometary ice.

Stephen Price (UCL, London, UK) talked of experimental studies of recombination reactions on interstellar surfaces.

Chemistry on surface of ices.

Debbie Waller (*U. Cambridge, UK*) talked on her experiments regarding ice growth in a cryo-ESEM microscope,

Hauke Trinks (*TU Hamburg, Germany*) discussed his findings on sea ice as a possible origin of life, based on his research expeditions to Spitsbergen.

Perspectives of Ice research and General Discussion and Conclusions

The meeting concluded with a discussion aimed at reviewing what had been learnt, and highlighting areas with special potential for future progress. The conclusions are discussed in the following section.

Assessment of the Results

The aim of bringing together specialists from different fields working in ice research with a view to stimulating exchanges was certainly achieved. The longer-term goal of lasting collaborations, we must, by definition, wait to find out whether it will be brought about by this meeting, but the signs so far are certainly encouraging, as the participants of the meeting are writing together an article designed to present the perspectives for future research on ice.

This perspectives article is presently in the form of a first draft, and it is planned that it will go through two or three iterations before being submitted for publication at some a review journal yet to be decided. Meeting funds have been reserved for the publication in case the authors decide to send it to a journal requiring publication fees.

The participants are also exploring the possibilities of further meetings and more interaction through applying for ESF and/or EU funds.

Another consequence of this meeting was his visibility in press and other Media, including live-interview for radio, news in local and national newspaper and in international magazines. This fact has contributed to the increase of visibility of the ESF and University of Granada to the European public and to the popularization of science.

Final WORKSHOP PROGRAMME

Wednesday 1st October 2008

Afternoon/evening *arrival*
20.00 *Welcome reception and Dinner*

Thursday 2nd October 2008

09.00-09.15 **Reception and welcome to the participants**

09.15-09.30 **Opening of EUROICE2008**
C. Ignacio Sainz-Díaz, Julyan Cartwright

09.30-09.50 **Presentation of the European Science Foundation (ESF)**
Hefin Jones (Standing Committee for Life, Earth and Environmental Sciences - LESC)

Session 1: Morphology and crystal growth of ices
Chair: Ignacio Sainz-Díaz (IACT, CSIC-UGR, Granada, Spain)

09.50-10.30 **Sea-ice and the origin of Life**
Hauke Trinks (Technische Universität Hamburg-Hamburg, DE)

10.30-11.10 **Morphology and properties of terrestrial ices**
Vance Bergeron (ENS, Lyon, France)

11.10-11.40 *Coffee break*

11.40-12.20 **IR and Raman spectroscopy of Ice from ab initio molecular dynamics**
Davide Donadio (University of California in Davis, USA)

12.20-13.00 **Stacking-faulty crystal structure of cubic ice and transformations.**
Werner F. Huhs (University of Gottingen, Germany)

13.00-13.40 **Applications of Cryo Environmental Electron Microscopy**
Debbie Stokes (FEI Instruments, NL)

13.40-16.00 *Lunch (Carmen de la Victoria)*

Session 2: Modeling of ice structures and properties
Chair: Rafael Escribano (Instituto de Estructura de la Materia, CSIC, Madrid, Spain)

16.00-16.40 **The shapes of icicles, growing and melting**
Raymond Goldstein (DAMPT, University of Cambridge, UK)

16.40-17.20 **Modelling of ice and water structures**
Emilio Artacho (Dept. of Earth Sciences, University of Cambridge, UK)

17.20-18.00 **Interaction of Ice on phyllosilicate surfaces by quantum mechanical calculations.** **Alfonso Hernández-Laguna** (EEZ, CSIC, Granada, Spain)

18.00-18.30 *Coffee break*

Session 3: Surface of ices and climate change
Chair: Ignacio Sainz-Díaz (CSIC, Granada)

18.30-19.10 **Geophysical models of sea-ice for the numerical investigations of climate.** **Jari Haapala** (Finnish Institute of Marine Research, Helsinki, Finland)

19.10-19.50 **Ice in the Upper Troposphere - Microphysics and Climate Effects**
Jan Pettersson (University of Gothenburg, Sweden)

19.50-20.30 **Morphology of ices in extreme conditions**
Julyan Cartwright (IACT, CSIC-UGR, Granada, Spain)

20.30 *Dinner*

21.30 *Cultural activity (Night visit to Alhambra Palace)*

Friday 3rd October 2008

Session 4: Spectroscopy of ices

Chair: **Alfonso Hernández-Laguna** (EEZ, CSIC, Granada, Spain)

- 09.00-09.40 **Inter and Intra Molecular Vibrations of Nitric Acid Hydrates**
Hinrich Grothe (Vienna University of Technology, Austria)
- 09.40-10.20 **Laboratory study of ices of cometary relevance: H₂O/CO₂, CO₂/HCH₃O**
Rafael Escribano (Instituto de Estructura de la Materia, CSIC, Madrid, Spain)
- 10.20-11.00 **Solid state solvation and ionization of HNO₃ on/in water clusters and ice: Dynamics and spectroscopy**
Nevin Uras-Aytemiz (Suleyman Demirel University, Isparta, Turkey)
- 11.00-11.30 *Coffee break*

Session 5: Physics of ices

Chair: **Julyan Cartwright** (IACT, CSIC-UGR, Granada, Spain)

- 11.30-12.10 **Order and disorder in ice structures**
John Finney (University College London, London, UK)
- 12.10-12.50 **Is there an HDA-LDA ice transition in 2D?**
Oreste Piro (Universidad de Islas Baleares, Mallorca)
- 12.50-13.30 **Crystal growth of ice in a Cryo-ESEM**
Debbie Waller (Cavendish Laboratory, Cambridge, UK)
- 13.30-15.30 *Lunch*

Session 6: Astrophysics and ices

Chair: **Oreste Piro** (Universidad de Islas Baleares, Mallorca)

- 15.30-16.10 **Physico-chemical properties of astrophysical ices**
Gianni Strazzulla (INAF, Italy)
- 16.10-16.50 **Experimental studies of recombination reactions on interstellar surfaces.** **Stephen Price** (UCL, London, UK)
- 16.50-17.30 *Coffee break*

Session 7: European Perspectives of Ice research

Chairs: **C. Ignacio Sainz-Díaz**, **Julyan Cartwright**

- 17.30-19.30 **General Discussion, future activities and Conclusions**
- 19.30-21.30 *Conference Dinner and Closure*

Saturday 4 October 2008

Morning *Departure*

Statistical Information

Age structure

35 – 45: 9

45 – 55: 4

55 +: 5

Sex

Female: 3

Male: 17

Countries of origin

Austria: 1

Finland: 1

France: 1

Germany: 2

Italy: 1

Netherlands: 1

Spain: 5

Sweden: 1

Turkey: 1

UK: 5

USA: 1

List of participants

Dr. Hinrich Grothe
Institute of Materials Chemistry
Vienna University of Technology
Veterinaerplatz 1/GA
1210 Vienna, Austria
Email: grothe@tuwien.ac.at
Tel. +43-1250773809
Fax: +43-1250773890

Prof. Giovanni Strazzulla
Osservatorio Astrofisico di Catania
Istituto Nazionale di Astrofisica
Via Santa Sofia 78
95123 Catania, Italy
Email: gianni@oact.inaf.it
Tel. +39-0957332315
Fax: +39-095330592

Prof. Stephen Price
University College of London
London, UK
Email: s.d.price@ucl.ac.uk
Tel: +44-2076794606
Fax: +44-2076797463

Prof. Jan Pettersson
Department of Chemistry
University of Göteborg
Kemivägen 10.
41296-Göteborg, Sweden
Email: janp@chem.gu.se
Tel. +46-317722828
Fax: +46-317723107

Dr. Debbie Stokes
Market Development Manager
NanoResearch Market Division
FEI Company
PO Box 80066
5600 KA EINDHOVEN
The Netherlands
E-mail: Debbie.Stokes@fei.com
Tel: +31 6 22 55 99 37
Fax: +31 40 23 567 64

Dr. Davide Donadio
Dept. of Chemistry
University of California at Davis
One Shields Ave.
Davis, CA 95616, USA
Email: ddonadio@ucdavis.edu
Tel: +1 530 752 2297

Dr. Jari Haapala
Finnish Institute of Marine Research
Erik Palmenin aukio 1,
P.O. Box 2
00561 Helsinki, Finland
email: Jari.Haapala@fimr.fi
tel: + 358 9 613 94 406 or + 358 40 757 3621
Fax : + 358 9 323 2970

Dr. Nevin Uras-Aytemiz
Department of Chemistry
Suleyman Demirel University
32260-Isparta, Turkey
Email: aytemiz@fef.sdu.edu.tr
Tel: +90 246 211 4114 |
Fax: +90 246-237 1106

Prof. Emilio Artacho
Department of Earth Sciences
University of Cambridge
Downing Street
Cambridge CB2 3EQ, UK
Email: emilio@esc.cam.ac.uk
Tel: (+44/0) 1223 333480,
Fax: (+44/0) 1223 333450

Prof. Raymond E. Goldstein
Department of Applied Mathematics and Theoretical Physics (DAMTP)
University of Cambridge,
Wilberforce Road
Cambridge, CB3 0WA, UK
Email: R.E.Goldstein@damtp.cam.ac.uk
Tel: +44-1223337908
Fax: +44-1223765900

Prof. John Finney
University College of London
London, UK
Email: john.finney@ucl.ac.uk
Tel: +44 (0)20 7679 7850
Fax: +44 (0)20 7679 0595

Dr. Debbie Waller
Department of Physics
Cavendish Laboratory,
University of Cambridge,
JJ Thomson Avenue
Cambridge CB3 0HE, UK
Email: dw284@cam.ac.uk

Dr. Vance Bergeron
Ecole Normale Supérieure
Lyon, France
Email: vance.bergeron@ens-lyon.fr
Tel: 33-6-26.87.27.11
Fax: 33-4-72.72.80.80

Prof. Hauke Trinks
Technische Universität Hamburg-Harburg
Harburger Schlossstraße 20
21079 Hamburg, Germany
Email: Hauke.Trinks@gmx.de
Tel.: +49 40 42878 3476/3213
Fax: +49 40 42878 2382

Prof. Werner F. Kuhs
Chair of Crystallography
University of Göttingen
Goldschmidtstr. 1
37077 Göttingen
Germany
Email: wf.kuhs@geo.uni-goettingen.de
Tel. +49 (0)551 393891
Fax +49 (0)551 399521

Prof. Rafael Escribano
Instituto de Estructura de la Materia, CSIC
C/ Serrano 123
28006-Madrid, Spain
Email: rescribano@iem.cfmac.csic.es
Tel: (34) 915901609
Fax: (34) 915855184

Dr. Alfonso Hernández-Laguna
Estación Experimental del Zaidín, CSIC
C/ Profesor Albareda, 1
18008-Granada, Spain
Email: alfonso@eez.csic.es
Tel: +34-958181600 (ext. 308)
Fax: +34-958129600

Prof. Oreste Piro
Department of Physics
Universitat de les Illes Balears
Campus Universidad
07122-Palma de Mallorca, Spain
Email: piro@imedea.uib.es
Tel. +34-971173230
Fax : +34-971173426

C. Ignacio Sainz-Díaz
e-mail: cisainz@ugr.es
Instituto Andaluz de Ciencias de la Tierra (IACT)
CSIC- Universidad de Granada
Edificio Instituto López Neyra
Av. del Conocimiento s/n
Parque Tecnológico de Ciencias de la Salud
18100-Armilla
Granada, Spain
Tel. 34-958-181644, Fax: 34-958-181632

Julyan Cartwright
e-mail: julyan@lec.csic.es
Instituto Andaluz de Ciencias de la Tierra, CSIC
Universidad de Granada
Av. Fuentenueva s/n
18002-Granada, Spain
Tel. 34-958-181644, Fax: 34-958-181632