

International Workshop Water X: exotic properties of water in extreme conditions

La Maddalena, 3-8 June 2018



Invited speakers:

- E. Backus, Max Planck Institute for Polymer Research, Mainz
- F. Caupin, Institute of Light and Matter, Lyon University
- G. B. De Giudici, Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari
- G. Franzese, Departament de Física de la Materia Condensada, Universitat de Barcelona
- G. Galli, Institute for Molecular Engineering, University of Chicago
- A. Goncharov, Geophysical Laboratory, Carnegie Institute of Washington
- S. Klotz, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, UPMC
- P. Launois, Laboratoire de Physique des Solides, Université Paris Sud
- N. Levinger, Department of Chemistry, Colorado State University
- J. Loveday, Institute for Condensed Matter and Complex Systems, The University of Edinburgh
- L. Michot, Laboratoire PHENIX, UPMC
- V. Molinero, Department of Chemistry, The University of Utah
- M. A. Ricci, Dipartimento di Scienze, Università degli Studi Roma Tre
- G. Schirò, Institut de Biologie Structurale, Grenoble
- A. K. Sum, Chemical and Biological Engineering Department, Colorado School of Mines
- J. Teixeira, Laboratoire Léon Brillouin, CEA Saclay

Sponsors:



Organizers:

L.E. Bove, CNRS & Sapienza Università di Roma
F. Bruni, Università Roma Tre
A. Desmedt, Université Bordeaux

WELCOME

We are pleased to welcome you for the 3rd edition of the WaterX: Exotic properties of water under extreme conditions workshop at the “Circle Ufficiali della Marina” in La Maddalena, Sardinia.

This event brings together leading experimental, theoretical, and computational scientists from among the unusually broad community of researchers interested in water physics and chemistry under extreme conditions, where extreme reads from deep supercooled regimes to very high or negative pressures, ultrashort time scales, extreme confinement, hydrates, etc. There are attendees representing physics, chemistry, earth and atmospheric science, and biology.

In the wonderful scenario of one of the most beautiful island of Mediterranean Sea, the workshop will provide an intimate context for learning the state of the art in the field and make connections across disciplines.

Wishing you a very nice and scientifically effective stay in Sardinia!

The organizing committee

Livia Eleonora Bove, CNRS-Univ. Pierre et Marie Curie & Università La Sapienza, Roma

Fabio Bruni, Università Roma III

Arnaud Desmedt, ISM CNRS - Univ. Bordeaux

Scientific Committee

Christiane Alba-Simionesco - LLB Saclay, France

Marc Johnson - ILL Grenoble, France

Werner Kuhs - Goettingen University, Germany

Claudio Masciovecchio - Elettra, Italy

Francesco Sciortino - Sapienza University, Italy

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PROGRAM OVERVIEW and INFORMATION

The scientific program will include 5 types of oral contribution:

- *Plenary* : 45 minutes (including 10 min discussions)
- *Keynote* : 30 minutes (including 5 min discussions)
- *Oral contribution* : 20 minutes (including 5 min discussions)
- *Short contribution* : 10 minutes (including 2 min discussions)
- *Flash contribution* for poster presentation) : 3 minutes

Some practical information for your stay and the social program:

- Please be aware that the workshop, lunches, coffee breaks and aperitifs will take place at the Marine Officer's Club, where a dressing code is requested. Of course you can dress casually but shorts, flip-flops, and teard jeans are forbidden in the Club's rooms.
- For the Caprera or Tahiti Trail participants, please don't forget to bring your sneakers or running shoes. The trail can be slippery.
- For the boat trip, please don't forget cap, sun cream, and of course your swimsuit!
- The island can be windy and the nights rather fresh, don't forget a K-way!

Timetable:

Sunday June 3											
time		time		time		time		time		time	
19:30	Welcome Cocktail										
time	Monday June 4 - Chair R. Saykally	time	Tuesday June 5 - Chair W. Kuhs	time	Wednesday June 6 - Chair A. Goncharov	time	Thursday June 7 - Chair C. Alba Simionescu	time	Friday June 8 - Chair TBC		
8:30	Opening & Registration	7:00	Sunrise Trail to Tahiti #	9:00	A. Sum	8:30	V. Molinero	7:00	Sunrise Scuba Diving **		
9:00	J. Teixeira	9:00	G. Galli					9:00	E. Backhus		
9:45	F. Caupin	9:45	A. Goncharov	9:45	J. Loveday	9:15	N. Levinger	9:45	A. Berger		
10:15	R. Grisenti	10:15	J. M. Brown	10:15	U. Ranieri	9:45	S. Meloni	10:05	B. Chazallon		
10:35	A. Angell	10:35	C. Q. Sun	10:35	F. Finocchi	10:05	B. Rossi	10:25	P. Giura		
10:55	A. Anisimov	10:55	F. Mouhat	10:55	R. Gaal	10:25	L. Tavagnacco	10:35	F. Formisano		
11:15	Coffee Break	11:05	Coffee Break	11:05	Coffee Break	10:35	Boat Excursion ##	10:45	Coffee Break		
11:35	P. Launois	11:30	S. Klotz	11:30	R. Saykally			11:05	G. De Giudici		
12:05	W. Schranz	12:00	C. Salzmann	12:00	H. J. Bakker			11:35	N. Ganfoud		
12:25	M. Chaplin	12:20	A. Thöny	12:20	C. Petuya			11:55	B. Capone		
12:45	M. Belyanchikov	12:40	J. Espinosa	12:40	M. Lemaire			12:15	Discussion & Closing Remarks		
12:55	Discussion	12:50	Discussion	12:50	Discussion			13:00	End		
13:15	Lunch	13:10	Lunch & Free Time	13:10	Lunch						
14:30	T. Whale	15:40	Coffee Break	14:30	L. Michot						
15:00	W. Kuhs	16:00	G. Franzese	14:30	L. Michot	18:00	G. Schiro				
15:20	F. Pietrucci	16:30	P. Poole	15:00	T. Dufils	18:30	P. Gallo				
15:40	E. Sanz	16:50	P. H. Handle	15:20	B. Jourmeaux	18:50	L. Comez				
16:30	Excursion: Caprera Trail or Garibaldi Museum	17:10	J. Russo	15:40	Coffee Break	19:10	M. Paolantoni				
		17:30	F. Martelli	16:00	M. A. Ricci	19:20	C. Bottari				
		17:50	Break			19:30	Free Time				
20:00	Town Talk: F. Bruni	18:00	Flash Presentations	16:30	R. Shi	20:15	Bus to Social Dinner				
		18:50	Apero-Poster	16:50	A. Di Cicco						
				17:10	V. Castiglio						
				17:30	Discussion						
				17:50	Punta Tegge Sunset Apéro *						

max 10 places available.

* An apero-dinner is available at Zi' Anto restaurant in Punta Tegge under request (price 25 €).

a local fee of 5 € will be requested when entering the 'Parco'.

** Scuba-diving will be operated by Best Shark Diving Center under request (Introductory lesson: price 10 €, 2h excursion: 55€).

DETAILED PROGRAM

Sunday, June 3

19:00 Registration

19:30 Welcome cocktail and Ice breaker.

Monday, June 4

08:30 Opening and registration

09:00 **Plenary. J. Teixeira** (LLB CNRS-CEA Saclay, France)

« *An experimentalist view of the properties of liquid water at low temperature.* »

09:45 **Keynote. F. Caupin** (ILM CNRS-Univ. Lyon, France)

« *Thermodynamic certainties and two-state speculations about the anomalies of water.* »

10:15 **R. Grisenti** (Helmholtz Institute Jena, Germany)

« *Probing intermolecular hydrogen bonds in supercooled water down to 230K.* »

10:35 **C. A. Angell** (Arizona State University, US)

« *Ideal solutions of ionic liquids and water in physics and biology.* »

10:55 **M. Anisimov** (Mariland University, US)

« *Resolving the Mystery of Heat- Capacity Anomalies Stemming from Hidden Liquid-Liquid Transitions in Pure Water.* »

11 :15 Coffee Break

11:35 **Keynote. P. Launois** (LPS CNRS – Univ. Paris Sud, France)

« *Water confined in hydrophilic and hydrophobic nanochannels: specific structural and dynamical properties.* »

12:05 **W. Schranz** (University of Vienna, Austria)

« *Glass freezing dynamics of confined water measured with DMA.* »

12:25 **M. Chaplin** (London South Bank University, UK)

« *The rebuttal of the 'Fourth phase of water' hypothesis with an osmotic hypothesis.* »

12:45 **M. Belyanchikov** (Moscow Institute of Physics and Technology, Russia)

« *Ferroelectricity of nanoconfined water molecules. Novel type of ferroelectric relaxors.* »

12 :55 Discussion

13:15 Lunch

14:30 **Keynote. T. Whale** (University of Leeds, UK)

« *Experimental routes to understanding heterogeneous ice nucleation.* »

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15:00 **W. Kuhs** (GZG University of Göttingen, Germany)

« *Emptying and refilling ice structures to explore extreme states of water for a better understanding of gas-water interactions.* »

15:20 **F. Pietrucci** (IMPMC CNRS – UPMC, Paris, France)

« *Towards a general approach to the simulation of structural transformations in water and other systems.* »

15:40 **E. Sanz** (Universidad Complutense de Madrid, Spain)

« *Understanding homogeneous ice nucleation with computer simulations.* »

16:00 *Break*

16:30 *Excursion: Caprera Trail or Garibaldi Museum*

20:00 **Town Talk (Sala Consolare at the City Hall). F. Bruni** (Università Roma III)

« *Cuocere quanto basta...ma quanto basta?* »

Tuesday, June 5

07:00 *Sunrise trail to Tahiti*

09:00 **Plenary. G. Galli** (University of Chicago, US)

« *Ab initio spectroscopy and ionic conductivity of water under extreme conditions.* »

09:45 **Keynote. A. Goncharov** (Carnegie Institution of Washington, US)

« *Water at high pressures.* »

10:15 **J.M. Brown** (University of Washington, US)

« *The Water-Carbon Dioxide System at High Pressure.* »

10:35 **C.Q. Sun** (Nanyang Technological Univ, Singapore)

« *Compression resolved mysteries of water, ice, and salt solutions.* »

10:55 **F. Mouhat** (UPMC Paris, France)

« *Excess proton dynamics in the protonated water hexamer: new insights from Quantum Monte Carlo calculations.* »

11:05 *Coffee Break*

11:30 **Keynote. S. Klotz** (IMPMC CNRS – UPMC, Paris, France)

« *Neutron studies on pure and salty ices VII & VIII: The good, the bad, and the ugly.* »

12:00 **C. Salzman** (University College London, UK)

« *New advances in the experimental exploration of water's phase diagram.* »

12:20 **A. Thoeny** (University Innsbruck, Austria)

« *Probing hydrogen ordering and disordering in ice VI proxies through librational Raman bands.* »

12:40 **J. Espinosa** (Universidad Complutense de Madrid, Spain)

« *Phase boundaries, nucleation rates and speed of crystal growth of the water-to-ice transition under an electricfield: a simulation study.* »

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12 :50 **Discussion**

13:10 *Lunch & Free Time*

15:40 *Coffee Break*

16:00 **Keynote. G. Franzese** (Univ. Barcelona, Spain)

« *Polymorphism, hexatic phases and polyamorphism in confined water.* »

16:30 **P. Poole** (St. Francis Xavier University, Canada)

« *Thermodynamic and structural anomalies of water nanodroplets.* »

16:50 **P.H. Handle** (Sapienza University of Rome, Italy)

« *Potential Energy Landscape of TIP4P/2005 water.* »

17:10 **J. Russo** (University of Bristol, UK)

« *Water-like anomalies as a function of tetrahedrality.* »

17:30 **F. Martelli** (IBM, UK)

« *Searching for ice-domains in amorphous ices.* »

17:50 *Break*

18:00 **Flash presentations** (see list of posters).

18:50 **Poster session** (see list of posters).

Wednesday, June 6

09:00 **Plenary. A. Sum** (Colorado School of Mines, US)

« *The Role of Water and Guests in the World of Gas Hydrates at Extreme Conditions.* »

09:45 **Keynote. J. Loveday** (University of Edinburgh, Scotland)

« *Water mixtures at modest pressures and temperatures.* »

10:15 **U. Raniery** (ILL, Grenoble, France)

« *Methane Dynamics in Ice Clathrates and Hydrates under High Pressure.* »

10:35 **F. Finocchi** (INSP CNRS – UPMC, Paris, France)

« *Structural and dynamical properties of methane hydrate under high pressure via Raman spectroscopy and first-principles molecular dynamics including nuclear quantum effects.* »

10:55 **R. Gaal** (EPFL, Lausanne, Switzerland)

« *Hydrogen bond symmetrization in ices and gas hydrates.* »

11:05 *Coffee Break*

11:30 **Keynote. R. Saykally** (University of California, US)

« *Reversed interfacial fractionation of carbonate and bicarbonate evidenced by X- ray photoemission spectroscopy.* »

12:00 **H. J. Bakker** (AMOLF, Amsterdam, Netherlands)

« *The Surface of Ice Is Like Supercooled Liquid Water.* »

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12:20 **C. Petuya** (ISM CNRS – Univ. Bordeaux, France)

« *Molecular gas selectivity study within mixed CO₂, CO and N₂ gas hydrates by Raman spectroscopy.* »

12:40 **M. Lemaire** (PhLAM CNRS-Univ. Lille, France)

« *Vapor deposition of nitrogen and water at low temperature (80- 130K) and under 1 bar: the extreme conditions of Enceladus environment.* »

12 :50 **Discussions**

13:10 *Lunch & Free Time*

14:30 **Keynote. L. Michot** (Phenix CNRS – UPMC, Paris, France)

« *Structure and dynamics of water in swelling clay minerals.* »

15:00 **T. Dufils** (LPTMC CNRS – UPMC, Paris, France)

« *The shape of water in magmatic liquids by molecular dynamics simulations.* »

15:20 **B. Journaux** (NASA Astrobiology Institute, Univ. Washington, US)

« *Experimental ice III, ice V and ice VI PVT equation of state measured in-situ, equilibrium with aqueous solution and implication for extraterrestrial ocean worlds.* »

15:40 *Break*

16:00 **Keynote. M.A. Ricci** (Univ. Roma, Italy)

« *The putative liquid-liquid transition in confined water is a liquid-ice transition.* »

16:30 **R. Shi** (Univ. Tokyo, Japan)

« *Impact of Salt Ions on the Structure and Dynamics of Water: Insight from a New Microscopic Structural Descriptor* »

16:50 **A. Di Cicco** (Physics Division Camerino, Italy)

« *Hydration Properties of the Zn²⁺ Ion in Water at High Pressure.* »

17:10 **V. Cristiglio** (ILL, Grenoble, France)

« *Monitoring of protein interactions in frozen and freeze-dried solution states using small angle scattering techniques.* »

17:30 **Discussion**

17:50 *Punte Tege Sunset Aperero*

Thursday, June 7

08:30 **Plenary. V. Molinero** (University of Utah, US)

« *Molecular Recognition of Ice by Proteins: from Ice Nucleation to Antifreeze.* »

09:15 **Keynote. N. Levinger** (Colorado State University, US)

« *Sweet confinement: interaction of carbohydrates with water in reverse micelles.* »

09:45 **S. Meloni** (Sapienza University of Rome, Italy)

« *Bubble Nucleation in Water Under Extreme Confinement: Modular Design of Hydrophobic Textured Surfaces to Enhance Self- Recovery of the Cassie- Baxter State.* »

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10:05 **B. Rossi** (Elettra - Sincrotrone Trieste, Italy)

« *Water-polymer interactions in nanopores of cyclodextrin- based hydrogels.* »

10:25 **L. Tavagnacco** (Sapienza University of Rome, Italy)

« *Water dynamics at low temperatures by confinement in PNIPAM microgels.* »

10:35 *Break*

11:00 *Boat Excursion*

18:00 **Keynote. G. Schirò** (IBS CNRS Grenoble, France)

« *Dynamical interplay between proteins and their hydration layer.* »

18:30 **P. Gallo** (Sapienza University of Rome, Italy)

« *Structure and dynamics of supercooled hydration water in biosolutions.* »

18:50 **L. Comez** (IOM-CNR, Italy)

« *NanoDNA sequences in water solutions: Structural and thermodynamic results in native and complexed samples.* »

19:10 **M. Paolantoni** (Università degli Studi di Perugia, Italy)

« *Water-like dynamics of formamide in aqueous mixtures.* »

19:20 **C. Bottari** (Elettra - Sincrotrone Trieste, Italy)

« *Solvation mechanism in Ionic Liquid – water mixtures: a theoretical and experimental UV Resonant Raman investigation.* »

19:30 *Free time*

20:15 **Bus to Social Diner**

Friday, June 8

07:00 *Sunrise Scuba Diving*

09:00 **Plenary. E. Backhus** (Max Planck Institute, Germany)

« *Vibrational Relaxation of water at the Ice – Air Interface.* »

09:45 **A. Berger** (Carnegie Institution of Washington, US)

« *2D Raman–THz Spectroscopy of water and heavy water near the freezing point.* »

10:05 **B. Chazallon** (PhLAM CNRS-Univ. Lille, France)

« *Selectivity and guest partitioning in co₂/n₂ clathrate hydrates.* »

10:25 **P. Giura** (IMPMC CNRS – UPMC, Paris, France)

« *Crystal like behaviour of dense liquid water: implication of the hydrogen bond network.* »

10:35 **F. Formisano** (UPMC Paris, France)

« *Switching-off the collective dynamics of liquid water upon immersion of golden nanoparticles.* »

10:45 *Coffee Break*

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11:05 Keynote. G. De Giudici (Università di Cagliari, Italy)

« *Impact of anthropogenic activities on water and marine sediments: La Maddalena harbour and other case history in Sardinia.* »

11:35 N. Ganfoud (PHENIX - CNRS – Univ. Sorbonne, France)

« *Blue energy and desalination with nanoporous carbon electrodes: From molecular simulations to continuous models.* »

11:55 B. Capone (Università degli Studi di Roma Tre, Italy)

« *Nanoparticles for Water Sanitation.* »

12 :15 Discussion and Closing Remarks

13:00 End

LIST OF POSTERS

1. **M. A. Anisimov** « Revisiting the heat-capacity anomaly in supercooled water by high-resolution adiabatic calorimetry »
2. **M. Belyanchikov** « Relaxor behavior and ferroelectricity of nanoconfined water molecules. Experiment and modeling »
3. **R. Berthelard** « Viscosity in supercooled water/glycerol solutions »
4. **J. M. Brown** « High-Pressure “Death” of Aqueous Electrolytic Chemistry »
5. **J. M. Brown** « Equation of State for Water from MPa to near TPa Pressures »
6. **J. M. Brown** « Carbonic Acid Monohydrate »
7. **M. M. Conde** « A comparative study of thermodynamic equilibrium of water in solution with NaCl for different force fields »
8. **S. Desplanche** « Water under strong acidity conditions: towards superprotonic conductor based on clathrate hydrates »
9. **M. Di Gioacchino** « Trehalose as a bioprotectant of peptides: A neutron diffraction study »
10. **J. Hrubý** « Supercooled water accurately »
11. **D. Lesnicki** « Dynamics and structure of water at the CaF₂/aqueous solution interface »
12. **A. Makurenkov** « Ortho/Para-Ratio of Water Spinisomers in Extremely Diluted Solutions »
13. **C. Métais** « Investigations of the impact of silica media on gas trapping selectivity within CO₂-N₂ mixed hydrate »
14. **A. Rosu-Finsen** « The Dopant-Effect in Ice V/ XIII and Ice VI/XV »
15. **V. Soprunyuk** « On the similarity of the behaviour of water in nano-porous materials and biological systems at low temperatures »
16. **C. Q. Sun** « Molecular undercoordination resolved mysteries of water and ice »
17. **C. Q. Sun** « Hydrogen bonding (O:H-O) thermodynamics of water and ice »
18. **A. Tinti** « Intrusion and extrusion of water in hydrophobic nanopores »

NOTES

