WaterX
exotic properties of water under extreme conditions

Book of Abstracts

May 24-29, 2026

Organizers

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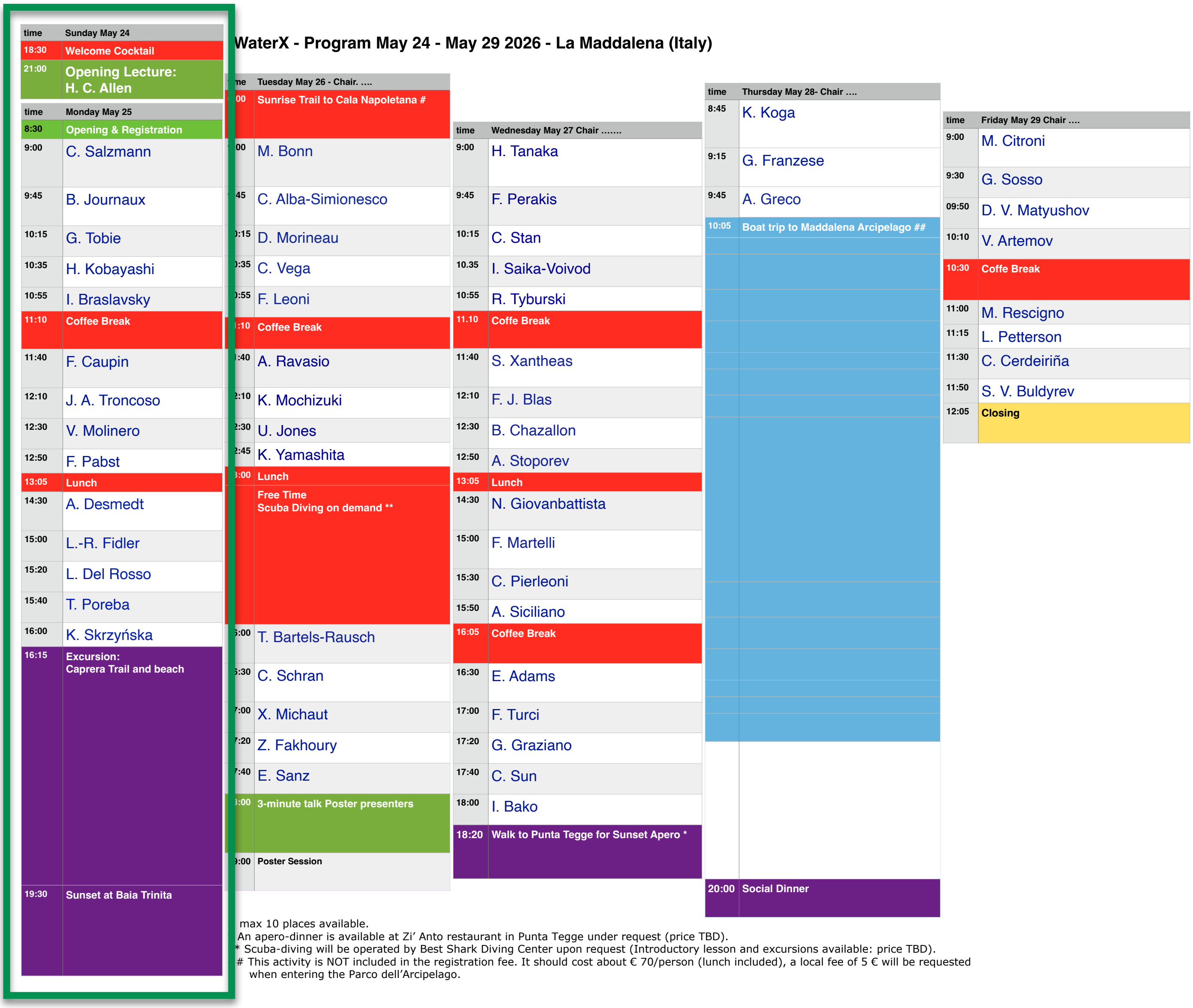
Venue

Circolo Ufficiali della Marina, Lungomare Ammiraglio Mirabello, 6 - 07024 La Maddalena (OT)
Maddalena Island, 07024 La Maddalena, Province of Olbia-Tempio, Sardinia (Italy)

Web Site

https://www.water-x.eu



WaterX - Program May 24 - May 29 2026 - La Maddalena (Italy)

time	Sunday May 24
18:30	Welcome Cocktail
21:00	**Opening Lecture: H. C. Allen**

time	Monday May 25
8:30	Opening & Registration
9:00	C. Salzmann
9:45	B. Journaux
10:15	G. Tobie
10:35	H. Kobayashi
10:55	I. Braslavsky
11:10	Coffee Break
11:40	F. Caupin
12:10	J. A. Troncoso
12:30	V. Molinero
12:50	F. Pabst
13:05	Lunch
14:30	A. Desmedt
15:00	L.-R. Fidler
15:20	L. Del Rosso
15:40	T. Poreba
16:00	K. Skrzyńska
16:15	Excursion: Caprera Trail and beach
19:30	Sunset at Baia Trinita

me	Tuesday May 26 - Chair. ....
00	Sunrise Trail to Cala Napoletana #
00	M. Bonn
45	C. Alba-Simionesco
:15	D. Morineau
:35	C. Vega
:55	F. Leoni
:10	Coffee Break
:40	A. Ravasio
:10	K. Mochizuki
:30	U. Jones
:45	K. Yamashita
:00	Lunch
	Free Time Scuba Diving on demand **
:00	T. Bartels-Rausch
:30	C. Schran
:00	X. Michaut
:20	Z. Fakhoury
:40	E. Sanz
:00	3-minute talk Poster presenters
:00	Poster Session

time	Wednesday May 27 Chair ....
9:00	H. Tanaka
9:45	F. Perakis
10:15	C. Stan
10.35	I. Saika-Voivod
10:55	R. Tyburski
11.10	Coffe Break
11:40	S. Xantheas
12:10	F. J. Blas
12:30	B. Chazallon
12:50	A. Stoporev
13:05	Lunch
14:30	N. Giovanbattista
15:00	F. Martelli
15:30	C. Pierleoni
15:50	A. Siciliano
16:05	Coffee Break
16:30	E. Adams
17:00	F. Turci
17:20	G. Graziano
17:40	C. Sun
18:00	I. Bako
18:20	Walk to Punta Tegge for Sunset Apero *

time	Thursday May 28- Chair ....
8:45	K. Koga
9:15	G. Franzese
9:45	A. Greco
10:05	Boat trip to Maddalena Arcipelago ##
20:00	Social Dinner

time	Friday May 29 Chair ....
9:00	M. Citroni
9:30	G. Sosso
09:50	D. V. Matyushov
10:10	V. Artemov
10:30	Coffe Break
11:00	M. Rescigno
11:15	L. Petterson
11:30	C. Cerdeiriña
11:50	S. V. Buldyrev
12:05	Closing

max 10 places available.

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

* Scuba-diving will be operated by Best Shark Diving Center upon request (Introductory lesson and excursions available: price TBD).

This activity is NOT included in the registration fee. It should cost about € 70/person (lunch included), a local fee of 5 € will be requested when entering the Parco dell'Arcipelago.

Aqueous Surface Electrostatics, Hydration, and Water Alignment informed by Surface Potential, Phase-Second Harmonic, and Interfacial and Bulk Spectroscopic Measurement: Phospholipids to Inorganic Ions

Heather C. Allen, Narendra Adhikari, Biswajit Biswas, Gwendolyn Nieto, Shamma Proma, Colin Bang
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Understanding how electrostatics and hydration shape interfacial structure is central to predicting membrane behavior, molecular recognition, and interfacial reactivity across biological and environmental systems including ocean/air and atmospheric aerosol/air interfaces. Here we retrieve electrical surface potential values from molecular-level phase – second harmonic generation to construct a coherent picture of charged air/aqueous interfaces. Using phase-sensitive second harmonic generation (phase-SHG), we quantify surface potentials (Φ_0) of lipid monolayers with distinct headgroup charged structures —cationic dimethyldioctadecyl ammonium bromide (DDAB, +24 mV), anionic 1,2-dipalmitoyl-sn-glycero-3-phosphoglycerol (DPPG, −27 mV), and zwitterionic 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC, −6 mV) — by separating intrinsic second-order ($\chi^{(2)}$) from field-dependent third-order ($\chi^{(3)}\Phi_0$) contributions, placing into perspective continuum model. The phase/amplitude analysis reveals that interfacial water orientation follows the net headgroup charge of phospholipids spread as surface films on water, albeit the values are surprisingly smaller in magnitude than surface potential values derived from vibrating plate and ionizing surface potential measurement methods. Scaling with Gouy–Chapman theory does not provide adequate explanation for the differing results.

In parallel, interface-selective vibrational sum frequency generation (VSFG), Raman, and infrared spectroscopy elucidate electrolyte hydration and speciation at the aqueous/air interface and in solution. Trivalent Al^{3+} from aqueous $AlCl_3$ exhibits longer-range interfacial influence relative to monovalent ions, with MD simulation (Hadi Dinpajooh, PNNL) revealing ion stratification, multilayering, and concentration-dependent compression (0.5–2.5 *m*). SSP/PPP-polarized VSFG OH intensities increase non-monotonically (0.5–1.5–2.5 *m*), robust to Fresnel corrections, indicating evolving interfacial depth and average water orientation consistent with stratification. Spectroscopy implicates a strong Al^{3+} hydration shell, acidity, solvent-shared ion pairing, and the hexaaqua complex in bulk.

Phospholipid film results show phase-SHG as a model-light, quantitative probe of Φ_0 and, when discussed in context with VSFG electrolyte data, provide a predictive framework in which net charge, ion-specific hydration/complexation, and water orientation collectively determine interfacial depth.

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[1] **Surface Potential of Phospholipid Monolayer Membranes Revealed by Phase-Sensitive Second Harmonic Generation,** Narendra M. Adhikari, Biswajit Biswas, Colin Bang, and Heather C. Allen, in Review 2.13.26.

[2} **Reorganization of Water at Aqueous Aluminum Chloride ($AlCl_3$) Interfaces: Vibrational Sum Frequency Generation and Molecular Dynamic Simulation;** Biswajit Biswas, Mohammadhasan Dinpajooh, Gwendolyn Nieto, Narendra Adhikari, Gregory K. Schenter, Shawn M. Kathmann, Christopher J. Mundy, Heather C. Allen, J. Phys. Chem. A 2025, 129, 46, 10616–10631. (OSU and PNNL)

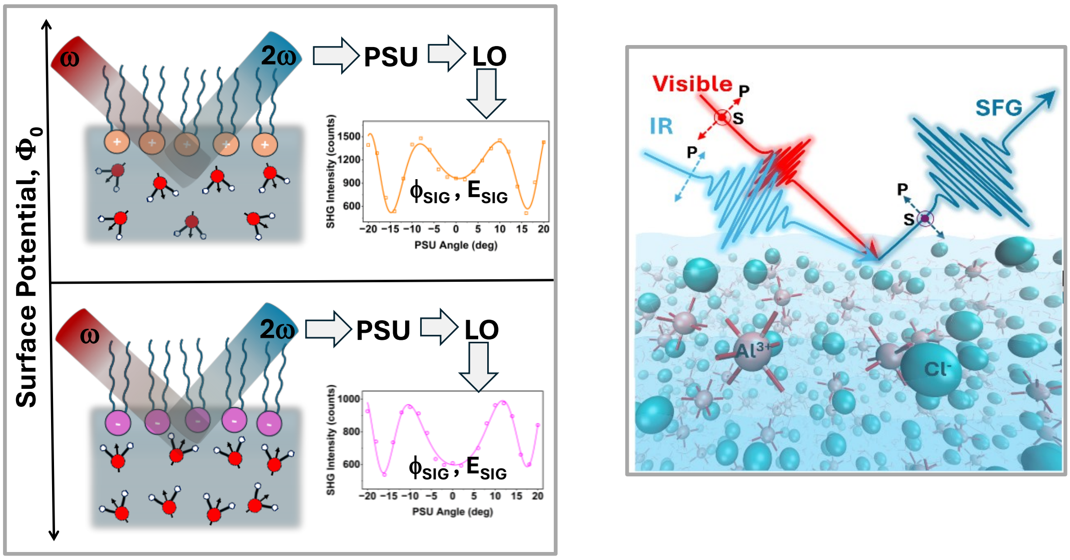

Figure 1. (a) Phase-second harmonic generation (Phase-SHG) derived surface potential values for phospholipid films on water reveal water alignment response to net surface charge density; the phosphate negative charge dominates in the zwitterionic DPPC. Phase-SHG provides a depth restricted (yet known depth) potential measurement. (b) Vibrational sum frequency generation (VSFG) spectroscopy reveal non-monotonic interfacial water structuring in aqueous $AlCl_3$ electrolyte solutions, driven by ion stratification and changes in water orientation with interfacial depth. These insights into trivalent ion behavior at aqueous interfaces have implications for environmental processes and aluminum-based energy storage technologies.

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Heterogeneous Nucleation and Interfacial Water Structure: From Atmospheric Microplastics to Heat-Battery Materials

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Heterogeneous nucleation and interfacial water structure play key roles in diverse natural and technological processes, ranging from ice crystallization in the atmosphere to energy storage in phase-change materials and the hydration of hydrophobic molecules.

In the atmospheric context, we examine the ice-nucleating ability of lab-made tire-wear particles,[1] one of the largest sources of microplastic pollution with global emissions approaching 6 Tg annually. Ice-nucleation experiments performed with our custom-built IceBox instrument demonstrate that tire-wear particles significantly elevate the freezing temperatures of supercooled water droplets, with activities between those of feldspar and quartz. Complementary new experiments investigate the ice-nucleating properties of textile fibers, providing insight into the potential atmospheric role of additional anthropogenic microplastic particles.

Nucleation processes are also critical for thermal-energy storage systems based on phase-change materials. Sodium acetate trihydrate (SAT) is a promising heat-storage material but exhibits strong supercooling. To identify effective nucleating agents, we developed the HeatMaster instrument, which enables parallel gram-scale analysis of phase transitions using power-compensation calorimetry. Screening of 36 candidate additives identified $CaCl_2{\cdot}2H_2O$ as the most effective nucleating agent, operating with remarkable thermal stability up to 80 °C.

Finally, we address the structural origins of hydrophobic hydration by examining the hydrophobic crossover using neutron diffraction.[3] Amorphous mixtures of water and anthracene were prepared by low-temperature vapour co-deposition to resolve the hydration structure around this hydrophobic "mini-graphene". The results reveal distinct structural motifs in the hydration shell, including water molecules with one broken hydrogen bond near the outer aromatic rings and partial dewetting at the central ring. These observations provide direct experimental evidence for structural changes associated with the hydrophobic crossover.

[1] Huh, Li, Gould, Whale, Salzmann, ACS EST Air 3 (2026) 449–456
[2] Li, Parkes, Salzmann, Cryst. Growth Des. 24 (2024) 8292-8300
[3] Madrigal, Vasilopanagos, Headen, Chikani, Rosu-Finsen, Pardo, Salzmann, chemRxiv (2026) 10.26434/chemrxiv.10001950/v1

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Water thermodynamic development tailored to extraterrestrial icy world's exploration: new invariant, novel hydrous phases and detectable signatures from space missions.

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The thermodynamic behavior of aqueous and hydrous systems at extreme conditions is central to understanding the outer solar system. Icy moons such as Europa, Ganymede, and Titan likely harbor the largest liquid water environments in the solar system: subsurface oceans in direct contact with ice Ih at the surface and with dense high-pressure polymorphs (ice II, III, V, and VI) at depth, where pressures exceed 200 MPa. Characterizing these systems is essential for constraining the physicochemical conditions any extraterrestrial life would need to tolerate.

Recent advances in high-pressure experimentation at planetary-relevant conditions, combined with geophysical modeling of icy worlds, have revealed new thermodynamic behaviors of aqueous solutions and hydrous solid phases. With major upcoming missions to Europa, Ganymede, and Titan prioritizing geophysical investigation, precise thermodynamic data for these systems are now critical inputs for mission science.

Here I review recent progress from a collaborative effort spanning the University of Washington, the European Synchrotron Radiation Facility, Texas A&M University, the Natural History Museum in London, the University of Nantes, and the Jet Propulsion Laboratory toward determining the thermodynamics of aqueous and hydrous phases at planetary conditions and interpreting their geophysical signatures on icy moons. In particular, I will focus on a new invariant defined in aqueous systems at high pressures: the cenotectic [1]; new equations of states for ices and aqueous solutions at extreme pressures [2], and novel hydrates and clathrate phase [3-5].

[1] Zarriz, A., Journaux, B., Powell-Palm, M.J., Nat. Comms. 2024 15, 10666.
[2] Journaux, B., et al. JGR-Planets 2020. 125, e2019JE006176.
[3] Journaux, B., et al. PNAS, 2023. 120, e2217125120.
[4] Pakhomova, A. et al., EPSL, 2025, 666, 119478.
[5] Collings, I.E., et al. ACS Earth Space Chem. 2026, 10 (2), 434-440

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New constraints on the composition and physical properties of the icy surface on Enceladus' South Polar Terrain

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The observation of active jets of ice grains and water vapour emanating from four warm faults (called tiger stripes) at Enceladus's South Pole was one of the major discoveries of the Cassini-Huygens mission [1,2,3,4]. Infrared mapping carried out by the Visual and Infrared Imaging Spectrometer (VIMS) on board the Cassini spacecraft provided information on surface composition, but also on the physical state (grain size and degree of crystallinity) near active faults [5,6,7,8,9,10]. However, many spectral characteristics were not fully exploited by previous studies. Here, by acquiring laboratory infrared spectra of ice powder analogues, we identified several salt compounds, and potentially CO_2 clathrate, at the surface, with a higher concentration along active faults. Our analysis shows that the spectral signatures in the inter-stripe regions are consistent with fresh, cold, fine-grained ice deposits, while ice near the tiger stripes has been thermally processed. The higher concentration of salts observed along the tiger stripes, as well as the main spectral features of water ice, imply significant sublimation and sintering processes in the vicinity of active jet sources. These new results provide essential constraints for identifying the best landing site for a future mission to Enceladus and for anticipating the mechanical properties of the icy regolith.

[1] C. Porco et al., 2006. Science, *311*(5766), 1393-1401; [2] J. Spencer et al. 2006, S*cience*, *311*(5766), 1401-1405; [3] J.H. Waite et al. 2006, *Science*, *356*(6334), 155-159; [4] F. Spahn et al. 2006, *Science*, *311*(5766), 1416-1418; [5] R. H. Brown et al. 2006, *Science*, *311*(5766), 1425-1428; [6] R. Jaumann et al. 2006, *Icarus*, *193*(2), 407-419; [7] C. Taffin et al. 2012, Planetary and Space Science, 61(1), 124-134; [8] Filachione et al. 2016, *Icarus*, *271*, 292-313; [9] J. P. Combe et al. 2019, *Icarus*, *317*, 491-508; [10] R. Robidel et al. 2020, *Icarus*, *349*, 113848.

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Predicted and unforeseen: On the identification of three metastable ice phases

Hiroki Kobayashi[1], Kazuki Komatsu[1], Kenji Mochizuki[2], Hayate Ito[1], Koichi Momma[3], Shinichi Machida[4], Takanori Hattori[5], Kunio Hirata[6], Yoshiaki Kawano[6], Saori Maki-Yonekura[6], Kiyofumi Takaba[6], Koji Yonekura[6,7], Qianli Xue[2], Misaki Sato[1], and Hiroyuki Kagi[1]

[1]Geochemical Research Center, Graduate School of Science, The University of Tokyo; [2]Department of Chemistry, Zhejiang University; [3]National Museum of Nature and Science; [4]Comprehensive Research Organization for Science and Society (CROSS); [5]J-PARC Center, Japan Atomic Energy Agency; [6]SPring-8 Center, RIKEN; [7]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University.

Metastable phases of ice rarely crystallise from water, thereby making it challenging to understand how they appear and where they can exist. We focus on deeply supercooled water as a good precursor state towards metastable ice phases. This was already well explored and known at ambient pressure, at which hyperquenching water or cooling emulsified water down to the homogeneous nucleation temperature (T_H) leads to the formation of stacking disordered ice (ice I_{sd}) with a high cubicity [1-2]. Through experiments using emulsified water, we found that a previously unknown phase (ice XXI) forms from supercooled water at T_H around 2.4 GPa. Around 1.2–1.5 GPa, the crystallisation of supercooled water at T_H yielded another previously unknown phase (ice XXII). Ice IV selectively forms between 0.45 and 1.1 GPa at T_H. Ice XXI can also be produced by heating emulsified high-density amorphous ice at 2.5 GPa. On cooling, ice XXI transforms into a hydrogen-ordered counterpart (ice XXIII). We faced a huge challenge in the structure analyses as they have very large unit cells ($V \sim 3000$ Å^3 and 6000 Å^3), but no single crystals were available due to the intrinsic limit of emulsions. We finally succeeded in solving the structures of all three phases employing powder x-ray and neutron diffraction, assisted by molecular dynamics (MD) simulations. Ice XXI has the structure of 'ice T2', a predicted phase by MD simulations [3]. This marks the very first experimental identification of a predicted high-pressure phase of ice. Also, what we proposed to name ice XXI is essentially the same as the recently reported ice XXI around 2 GPa by Lee *et al.*, discovered through a series of rapid compression experiments of liquid water at room temperature [4]. Through different approaches, it was thus shown that supercooled water preferencially crystallise into metastable phases. In this presentation, I will discuss (i) how we solved such highly complex structures based on powder diffraction methods, (ii) melting curves and metastability crossovers of metastable ice phases, and (iii) relevance to the crystal structure prediction [5].

[1] E. Mayer and A. Hallbrucker. *Nature.* 1987, **325**, 601–602.
[2] B. Murray, D.Knopf, and A. Bertram. *Nature*, 2005, **434**, 202–205.
[3] T. Yagasaki, M. Matsumoto, and H. Tanaka. *J. Phys. Chem. B*, 2018, **122**, 31, 7718–7725.
[4] Y.-H. Lee *et al. Nat. Mat.* 2026, **25**, 302–309.
[5] H. Kobayashi *et al. arXiv preprint*, 2025, arXiv:2507.14415.

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Atomic Force Microscopy of Ice Interfaces in Supercooled Water

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[b] Department of Earth and Planetary Sciences, Weizmann Institute of Science, Rehovot, Israel

Ice formation in aqueous systems governs processes ranging from cloud microphysics and environmental freezing to cryobiology and food preservation. However, the microscopic mechanisms controlling how particles, cells, and macromolecules interact with advancing ice fronts remain poorly understood. In particular, two fundamental questions persist: how particles become engulfed or rejected during freezing, and how biological molecules such as ice-binding proteins (IBPs) [1] regulate ice growth.

Here we introduce an experimental platform that combines low-temperature atomic force microscopy (AFM) [2] with inverted optical microscopy to investigate ice interfaces directly in supercooled water. This correlative approach enables simultaneous visualization of ice crystals and nanoscale interrogation of the ice surface under controlled subzero conditions. The optical channel tracks ice-front dynamics, particle motion, and fluorescence-labeled molecules during directional freezing, while AFM provides topographical and nanomechanical mapping of the ice interface with submicron resolution.

This capability allows investigation of particle engulfment by advancing ice fronts, including the conditions under which particles and cells are rejected, pushed ahead of the interface, or incorporated into the growing crystal. In parallel, we examine how ice-binding proteins adsorb to specific crystallographic planes and inhibit step propagation, thereby blocking ice growth and modifying crystal morphology. Together, these measurements establish a framework for studying water–ice–particle interactions and the biological regulation of ice growth in aqueous environments.

[1] M. Bar Dolev, I. Braslavsky, P.L. Davies, Ann. Rev. of Biochem. 2016, 85, 515-542

[2] M. Chasnitsky, S.R. Cohen, Y. Rudich, I. Braslavsky, J. of Cryst. Growth 2023, 601, 126961

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Dynamics of water under pressure: a cascade of anomalies

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Contrary to other liquids, the dynamics of water accelerates when pressure is applied, even at ambient temperature. The self-diffusion coefficient D increases, while shear viscosity η decreases, before they both reach extrema and recover a normal behavior at high pressure. The structural relaxation time τ also shows a decrease, but no minimum in the pressure range where measurements were available [1]. We have measured shear viscosity and sound attenuation in water at ambient temperature and up to 1. 6 GPa [2]. Our data on η allow to settle an existing discrepancy between conflicting measurements in the GPa range. In addition, a visco-elastic analysis [3] yields the relaxation time and elastic moduli of water, revealing that τ reaches a minimum around 500 MPa. All results are confirmed with molecular dynamics simulations of the TIP4P/2005 model [4], which provide additional microscopic insight about pressurized water. The minimum in relaxation time occurs in the same pressure range as another anomaly in the translational order of water, revealing a profound restructuration of the hydrogen bond network. The comprehensive picture that emerges is that of a cascade of structural, dynamic, and thermodynamic anomalies in water [5].

[1] F. Bencivenga, A. Cimatoribus, A. Gessini, M. G. Izzo, and C. Masciovecchio, J. Chem. Phys. 2009, 131, 144502.

[2] J Eichler, J Stefanski, JM Roca, I Daniel, B Issenmann, C Valeriani, and F. Caupin Phys. Rev. Lett. 2025, 134, 134101.

[3] L. Hall, Phys. Rev. 1948, 73, 775.

[4] J. Martín-Roca, A. Zaragoza, F. Caupin, and C. Valeriani. J. Chem. Phys. 2026, 164, 064501.

[5] J. R. Errington and P. G. Debenedetti, Nature 2001, 409, 318.

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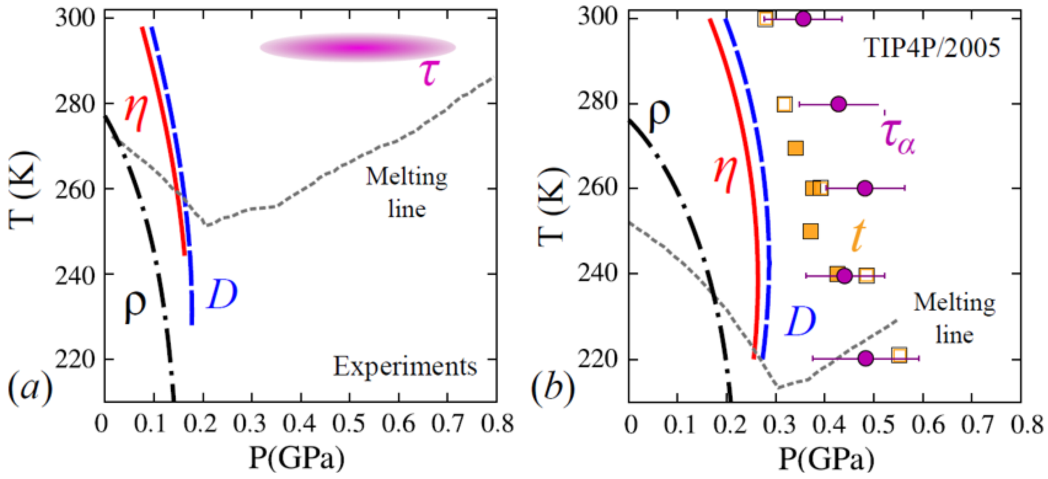

Line of anomalies in water for experiments (a) and TIP4P/2005 simulations (b).

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Experimental Density Measurements and Molecular Simulation of Supercooled LiCl, NaCl and KCl Aqueous Solutions

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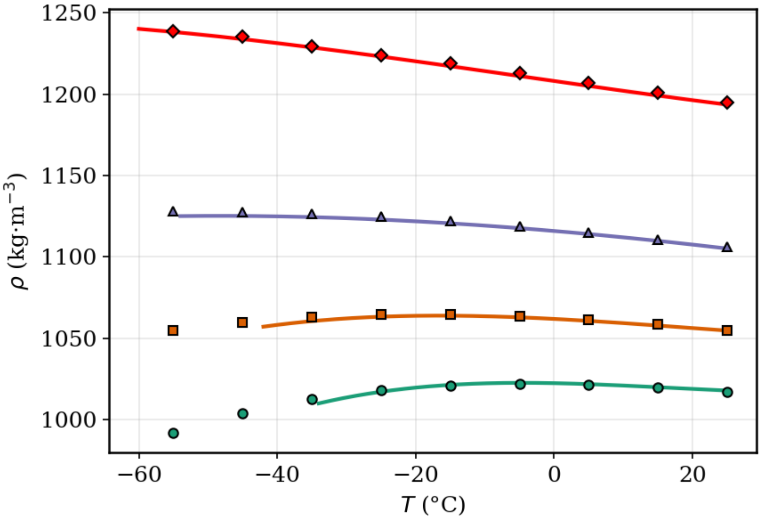
Density of supercooled aqueous solutions of lithium, sodium, and potassium chlorides has been experimentally determined at atmospheric pressure down to −60 °C within the room temperature solubility range using dilatometry. Solutions were dispersed within a hydrophobic matrix, forming an emulsion that strongly inhibits heterogeneous nucleation [1]. The temperature of maximum density and the apparent molar volume were calculated from density data. Molecular dynamics simulations were performed for these systems within the same concentration and temperature ranges using the Madrid-2019 force fields [2]. Experimental and simulation results show excellent agreement, which supports the use of Madrid-2019 to investigate the structure of these solutions. The structural analysis reveals that potassium and sodium exhibit rather similar structural features, whereas lithium shows a clearly distinct behavior, with water molecules arranged in a tetragonal configuration around the lithium ion resembling a solid-like structure.

[1] O. Mishima, J. Chem. Phys. 2007, 24, 244507.

[2] I. Zeron, J.L.F. Abascal, C. Vega, J. Comput. Phys. 2019, 151, 134504.



Density versus temperature for NaCl at different molalities. From bottom to top: 0.5, 1.5, 3, and 6 mol/kg. Lines are fits to experimental results and symbols are simulation data.

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Rethinking the Evidence for a Liquid-liquid Transition in Water

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The identification of a liquid–liquid transition (LLT) in supercooled water hinges on the ability to distinguish its structural signatures under experimentally accessible conditions. Ultrafast decompression experiments have interpreted the emergence of two peaks in the structure factor $S(q)$as evidence of distinct high-density (HDL) and low-density (LDL) liquids.[1-3] However, this interpretation is difficult to reconcile with the thermodynamic constraints of adiabatic decompression and the limited time available for structural evolution by the time these features are observed.

To understand the process and assist in the interpretation of the experiments, we performed large-scale molecular simulations of adiabatic decompression using ML-BOP,[4] a monatomic water model that exhibits a LLT.[5] We find that quasi-equilibrium adiabatic decompression from temperatures below $T_c$drives the system along the LLT, crossing the liquid–liquid critical point (LLCP) and subsequently evolving near the Widom line. In contrast, when decompression starts at or above T_c, the system does not cross the LLCP: the decompression trajectory is deflected to higher temperatures by the large heat capacity of the critical region.

Our simulations show that even when the system evolves along the LLT, the structure factor exhibits a single first strong diffraction peak because HDL and LDL domains remain nanoscopic. The combination of low HDL–LDL interfacial tension and the high viscosity of supercooled water prevents sufficient coarsening to produce distinct scattering features before crystallization intervenes. The two-peak signals observed experimentally can instead be explained by the superposition of contributions from regions of the sample evolving at different temperatures, consistent with the reported ~ 20K temperature gradients across ~ 40 μm samples in Ref. [1].

We identify the decisive structural signature of the LLT as the emergence of a domain peak at wavevectors below the experimentally accessible range, arising from nanoscopic phase separation along the LLT. Although this peak lies outside the measured q-window, its presence manifests indirectly as a transient increase in the apparent correlation length extracted from the low-q tail of $S(q)$, consistent with experimental observations.

[1] K. H. Kim et al., Science 370, 978–982 (2020).

[2] K. Amann-Winkel et al, Nat. Commun. 14, 442 (2023).

[3] S. You et al., Science 391, 1387–1391 (2026).

[4] R. Kumar, I. de Almeida Ribeiro, D. Dhabal, and V. Molinero, J. Chem. Phys. 164, 024506 (2026).

[5] D. Dhabal, R. Kumar, and V. Molinero, *PNAS.* **121**, e2322853121 (2024).

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Glassy Arrest Behind the Apparent Second Liquid in Water

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The origin of water’s anomalous behavior remains a central open problem in the physical sciences and is often attributed to a liquid–liquid transition (LLT) between high- and low-density liquid states deep in the supercooled regime. Experimental access to this region is hindered by rapid crystallization, leaving atomistic simulations as the primary source of supporting evidence. Using extensive machine-learning–accelerated first-principles simulations in direct comparison with spectroscopic, structural, and dynamical experimental measurements, we show that features commonly interpreted as signatures of an LLT can instead be explained by the onset of glassy dynamics. Specifically, we find that the fluctuations previously associated with an LLT [1,2,3] reflect a transformation from a high-density liquid to a kinetically arrested low-density glass. These results call for a reassessment of water’s metastable landscape, suggesting that many anomalies in the supercooled regime arise from a surprisingly high glass-transition temperature of ambient-pressure low-density water, 189±8 K—remarkably close to the temperature previously associated with the LLT.

[1] G. Debenedetti, F. Sciortino, G. H. Zerze, Second critical point in two realistic models of water. Science 369 (6501), 289–292 (2020).
[2] T. E. Gartner III, P. M. Piaggi, R. Car, A. Z. Panagiotopoulos, P. G. Debenedetti, Liquid-liquid transition in water from first principles. Phys. Rev. Lett. 129 (25), 255702 (2022).
[3] F. Sciortino, Y. Zhai, S. Bore, F. Paesani, Constraints on the location of the liquid–liquid critical point in water. Nature Phys. 21 (3), 480–485 (2025).

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Gas Hydrates in Water-Rich Systems: From Spectroscopy to Geosciences and Energy

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Gas hydrates are ice-like systems made of a network of hydrogen-bonded water molecules (forming host cages), stabilized by the inclusion of guest molecules [1]. Such water-rich systems are at the crossroads of major challenges related to water, energy, geosciences and climate [2]. A multiscale approach is required for understanding these systems, from molecular mechanisms to natural occurrences in geological environments (deep sea floor) through potential applications in energy (gas separation, storage, etc.) [3]. At the fundamental level, advanced experimental and computing techniques are employed to probe hydrate structures, guest–host interactions, dynamics and excitations, and cage occupancy under varying thermodynamics conditions. These approaches provide key insights into the stability and formation kinetics of hydrates, essential for predicting their behaviour in complex systems. The formation of gas hydrates in confined media such as clay-rich sediments, relevant to natural environments represents a key challenge nowadays. By investigating the role of mineral interfaces and chemistry, a better assessment of natural methane reservoirs and their potential climat impact is accessible. Beyond fundamental science, these studies open pathways toward innovative applications, including gas storage and transport, CO_2 capture and sequestration and selective gas separation processes. Such issues highlight the potential of hydrate-based technologies in the future developments.

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Self-Preservation of CO2 Hydrates: Gravimetric and Thermal Analysis

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We have utilized Simultaneous Thermal Analysis (STA) to investigate the dissociation of CO_2 hydrates in the self-preservation region upon heating from -80°C. This technique allows us to precisely monitor the degasification of small samples (< 60 mg) as a function of temperature. Furthermore, we have determined dissociation rates from isotherms at different temperatures between −70 °C and 0 °C.

Unlike reports on other gas hydrates, such as CH_4 hydrates, we reveal that CO_2 hydrates do not simply exhibit high dissociation rates below the self-preservation regime and low dissociation rates within [1,2]. Instead, two distinct dissociation steps occur: up to 13% of the hydrate dissociates between −60 and −40 °C, and the remainder dissociates above −15 °C. In between the two steps the dissociation rate decreases substantially, where a state of "self-preservation" is reached. Dissociation rates in the self-preservation zone are lower by a factor of 30 than below and 700 than above it.

After recooling from −20 °C to below −80 °C the first dissociation step appears again upon heating, i.e., the self-preservation condition can be deactivated by cooling. However, only about one quarter of the initial mass loss are recorded for the reactivated low-temperature dissociation. Assuming the ice shield theory to be correct our observation suggests that the ice shield forms between -60 and -40°C, but then partly breaks when recooling to -80°C. If the ice shield theory is incorrect then there is a process that is reversed upon cooling that allows to trigger dissociation.

The two-step behavior observed here has not been reported in previous studies using samples of 500 times larger masses or more [3–5]. This is likely due to the larger surface-to-volume ratio in small samples and supports the hypothesis that self-preservation is a surface-related effect.

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Unveiling the emptied hydrates: new insights from the intermediate pressure regime

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The study of the complex polymorphism of the solid mixture of water and gases at high pressure continues to yield exciting discoveries. In particular, several solid stoichiometric and non-stoichiometric phases of the mixture H_2O-H_2 have been characterized in the latest years [1], some of which, being metastable at ambient pressure and low temperature (i.e., 77 K), can be recovered and handled in laboratory. Surprisingly, three of them, i.e., sII clathrate as well as C_0 and C_2 hydrates, show a metastable behaviour even in the absence of a molecular guests in the water framework. Starting from different mother phases (i.e., sII and C_0) synthesized in an intermediate pressure regime (i.e., below 5 kbar), samples underwent a warming treatment in dynamic vacuum conditions, yielding in this way three pure ice polymorphs: XVI [2], XVII [3], and Ic [4,5]. Here, we report our studies concerning the synthesis and characterization of these hydrates and their emptied counterparts [6-9], mainly performed through Raman and neutron scattering experiments. We also discuss the properties of the other emptied hydrates studied to date (e.g., methane and nitrogen hydrates), in the new perspective of considering these materials as relevant for both technological applications [7] and the astrophysical context [10].

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Cryopreservation of hydrogen in crystalline cubic ice

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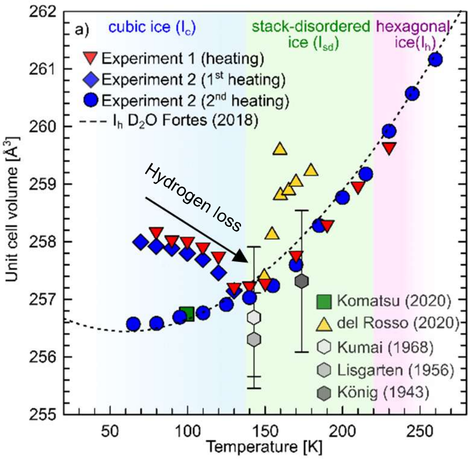

Figure 1. Unit cell volume evolution of cubic ice produced by decompression (to 0.1 MPa) of C_2 hydrogen hydrate at low temperature (red and blue symbols) determined by neutron diffraction.

We demonstrate that fully crystalline cubic ice (I_c), despite its non-porous structure, can retain molecular hydrogen as an interstitial guest following controlled decompression of a high-pressure hydrogen hydrate precursor. Hydrogen-rich filled-ice C_2 hydrate was synthesized above ~3 GPa and decompressed at cryogenic temperatures. Upon pressure release, the hydrate transforms topotactically into cubic ice while preserving the cubic symmetry of the parent phase. Synchrotron X-ray diffraction, neutron diffraction, and Raman spectroscopy reveal that the recovered cubic ice exhibits a reproducible lattice expansion relative to hydrogen-free ice, indicating the presence of residual hydrogen within the lattice. This expansion persists up to ~130 K at ambient pressure (Figure 1) and disappears upon heating, consistent with progressive hydrogen release. Raman spectroscopy provides independent evidence for hydrogen retention through characteristic rotational and vibrational modes. Quantitative analysis indicates that several percent of the hydrogen present in the parent hydrate remains trapped within the cubic ice framework. At moderate pressure (0.18 GPa), cubic ice can also partially re-incorporate hydrogen released during hydrate decomposition, producing measurable lattice expansion and demonstrating reversible hydrogen uptake. These results reveal an unexpected ability of a dense hydrogen-bonded crystal to host hydrogen without permanent porosity or chemical bonding, establishing cubic ice as a model system for hydrogen–lattice interactions and suggesting new pathways for hydrogen stabilization in molecular solids.

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Probing CH_4 and CO_2 Clathrate Hydrates at Their Extremes via Single-Crystal X-ray Diffraction

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CH_4 clathrate hydrate is the subjects of intensive research, driven by its potential in energy industry and role in planetary interior modeling. However, the evolution of high-pressure CH_4 hydrate (MH-II) above 1.4 GPa has been the subject of active debate [1–3], with conflicting interpretations suggesting either a transformation to a new clathrate structure, changes in cage occupancies, or the coexistence of clathrate hydrate and filled ice. These discrepancies highlight a fundamental gap in our knowledge of the gas clathrate hydrates at conditions relevant to the interiors of exoplanets and icy moons. In this study, we investigate the high-pressure (HP) evolution of CH_4 hydrate using *in situ* single-crystal and powder X-ray diffraction in diamond anvil cells at the ID27 beamline of the European Synchrotron Radiation Facility (ESRF). We discovered a novel clathrate structure (denoted MH-IIb or sH-II, sp. group $P\bar{6}2m$ $a = 11.6203(1)$ Å; $c = 9.836(8)$ Å; $V = 1150.2(9)$ Å^3), stable between 1.44 GPa and 2.13 GPa, that has hitherto been unobserved in any hydrate system [4]. Our results demonstrate that pressure drives progressive filling of the clathrate cages, critically enhancing host–guest and guest–guest interactions and eventually leading to the phase transition associated with the methane–methane steric repulsion and formation of an unconventional $C-H\cdots O$ hydrogen bond. Our results indicate that the MH-IIb phase may serve as a methane reservoir in the outer part of the differentiating core of early Titan, thereby impeding degassing and accounting for the delay in the formation of Titan's methane-rich atmosphere.

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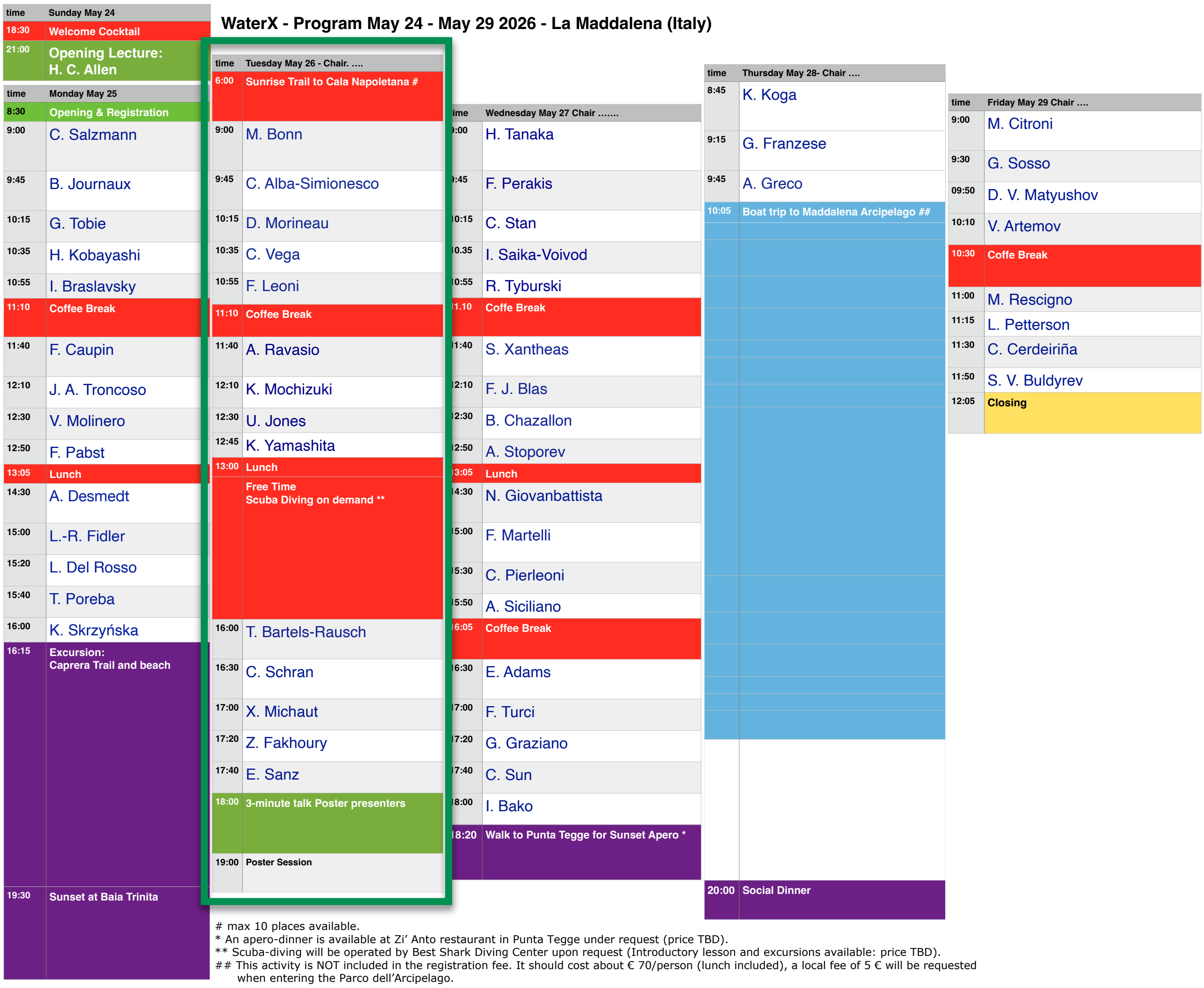

WaterX - Program May 24 - May 29 2026 - La Maddalena (Italy)

time	Sunday May 24
18:30	**Welcome Cocktail**
21:00	**Opening Lecture:** **H. C. Allen**

time	Monday May 25
8:30	**Opening & Registration**
9:00	C. Salzmann
9:45	B. Journaux
10:15	G. Tobie
10:35	H. Kobayashi
10:55	I. Braslavsky
11:10	**Coffee Break**
11:40	F. Caupin
12:10	J. A. Troncoso
12:30	V. Molinero
12:50	F. Pabst
13:05	**Lunch**
14:30	A. Desmedt
15:00	L.-R. Fidler
15:20	L. Del Rosso
15:40	T. Poreba
16:00	K. Skrzyńska
16:15	**Excursion:** **Caprera Trail and beach**
19:30	**Sunset at Baia Trinita**

time	Tuesday May 26 - Chair. ....
6:00	**Sunrise Trail to Cala Napoletana #**
9:00	M. Bonn
9:45	C. Alba-Simionesco
10:15	D. Morineau
10:35	C. Vega
10:55	F. Leoni
11:10	**Coffee Break**
11:40	A. Ravasio
12:10	K. Mochizuki
12:30	U. Jones
12:45	K. Yamashita
13:00	**Lunch**
	Free Time **Scuba Diving on demand ****
16:00	T. Bartels-Rausch
16:30	C. Schran
17:00	X. Michaut
17:20	Z. Fakhoury
17:40	E. Sanz
18:00	**3-minute talk Poster presenters**
19:00	**Poster Session**

ime	Wednesday May 27 Chair ....
:00	H. Tanaka
:45	F. Perakis
0:15	C. Stan
0.35	I. Saika-Voivod
0:55	R. Tyburski
1.10	**Coffe Break**
1:40	S. Xantheas
2:10	F. J. Blas
2:30	B. Chazallon
2:50	A. Stoporev
3:05	**Lunch**
4:30	N. Giovanbattista
5:00	F. Martelli
5:30	C. Pierleoni
5:50	A. Siciliano
6:05	**Coffee Break**
6:30	E. Adams
7:00	F. Turci
7:20	G. Graziano
7:40	C. Sun
8:00	I. Bako
18:20	**Walk to Punta Tegge for Sunset Apero ***

time	Thursday May 28- Chair ....
8:45	K. Koga
9:15	G. Franzese
9:45	A. Greco
10:05	**Boat trip to Maddalena Arcipelago ##**
20:00	**Social Dinner**

time	Friday May 29 Chair ....
9:00	M. Citroni
9:30	G. Sosso
09:50	D. V. Matyushov
10:10	V. Artemov
10:30	**Coffe Break**
11:00	M. Rescigno
11:15	L. Petterson
11:30	C. Cerdeiriña
11:50	S. V. Buldyrev
12:05	**Closing**

\# max 10 places available.
* An apero-dinner is available at Zi' Anto restaurant in Punta Tegge under request (price TBD).
** Scuba-diving will be operated by Best Shark Diving Center upon request (Introductory lesson and excursions available: price TBD).
\#\# This activity is NOT included in the registration fee. It should cost about € 70/person (lunch included), a local fee of 5 € will be requested when entering the Parco dell'Arcipelago.

Molecular Mechanics of Aqueous Interfaces from Surface Vibrational Spectroscopy

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Understanding how water, ions, and surfaces interact across length scales is central to electrochemistry, nanofluidics, and catalysis. In particular, the impact of hydrogen-bond network termination and interfacial charges on the arrangement of counterions and water has been the subject of intense debate. Across three studies, we have established a molecular-level picture of structure and dynamics at aqueous interfaces under confinement and electrostatic perturbation.

We have demonstrated that, down to the angstrom-scale confinement, interfacial effects entirely determine the organization of confined water, disrupting bulk-like hydrogen bonding and producing asymmetric environments due to wall contact [1]. These findings establish that nanofluidic behavior is governed not by the confined volume, but by its bounding interfaces. We extended this picture to show that even nominally neutral materials, such as hexagonal boron nitride, acquire a spontaneous surface charge at the aqueous interface [2]. This intrinsic charging, observed in other solids as well, indicates that the formation of an electric double layer (EDL) is nearly universal at solid–liquid boundaries. Finally, we resolved the ultrafast dynamics of the aqueous EDL using femtosecond-resolved optical spectroscopy, showing that ionic rearrangements occur within tens of picoseconds — faster than diffusion-limited models predict [3]. Together, these studies provide a molecularly consistent understanding of how interfacial polarization, confinement, and charge collectively define water's behavior in nanofluidic and electrochemical environments.

[1] Y. Wang et al., Nature Commun. 16, 7288 (2025).
[2] Y. Wang et al., J. Am. Chem. Soc. 147, 30107 (2025).
[3] A. Greco et al., Science 388, 405 (2025).

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Simplified Phase Behavior of Water under Nanoconfinement

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2. *Université Clermont Auvergne - Institut Pascal - Polytech Clermont Auvergne*
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Nanoconfinement—restricting water to nanoscale spaces such as nanopores, nanotubes, or interfaces—profoundly disrupts its hydrogen-bond network, altering its physical and chemical properties in unprecedented ways. This transformation challenges the conventional "bulk-like" behaviors of water and opens new avenues in materials science, biology, and nanotechnology. One of the most striking effects of nanoconfinement is the dramatic simplification of water's phase diagram. While bulk water exhibits up to 18 crystalline polymorphs depending on pressure and temperature conditions, nanoconfined water often displays only 2 or 3 crystalline phases—or none at all. This reduction arises from geometric constraints and surface interactions that inhibit nucleation and growth of conventional ice phases. Using neutron diffraction and thermodynamic measurements on a wide range of nanoporous materials with controlled pore sizes and surface chemistries, investigated across varying temperature and pressure conditions, we revisit the fundamental phase behavior of water under confinement—conditions ubiquitous in natural and technological systems.

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Confinement Effects on Water and Aqueous Solutions in Deeply Supercooled and Partially Frozen States

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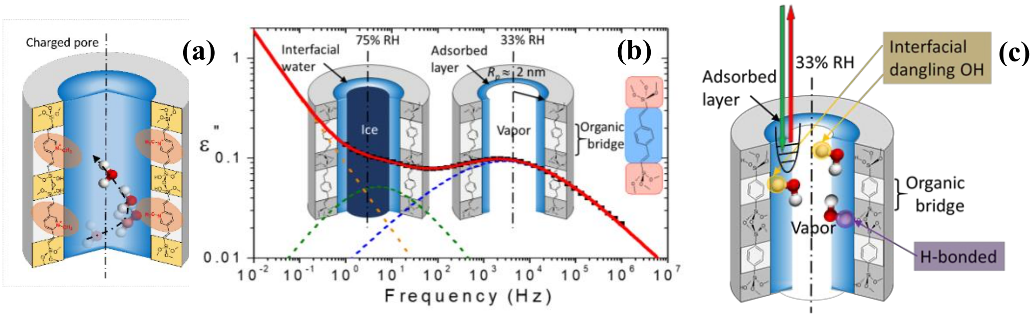
The nanometric confinement of water within pores dramatically alters its fundamental properties. By employing periodic mesoporous silicas and organosilicas (PMOs) featuring diverse organic bridging units, we finely modulated surface interactions—adjusting hydrophilicity and ionic surface charge. Here, we reveal the profound effects on water's structure and dynamics, including a huge slowdown of liquid mobility in charged pores. Additionally, we delve into the low-temperature phase behavior and ice-driven structural transformations in nanoconfined water-glycerol mixtures.



Sketches of the different configurations of water confined in PMOs as studied by (a) QENS [Mozhdehei 2025], (b) broadband dielectric spectroscopy [Malfait 2021], and (c) Raman spectroscopy [Malfait 2022].

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Learning physics by simulating electrolytes

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Simulations of electrolytes are challenging and typically involve explicit inclusion of water. The simplest approach is to use non-polarizable models for both water and ions. We shall present the current development of the Madrid-2019 force field, which utilizes the TIP4P/2005 model for water and scaled charges for the ions [1-5]. The model is simple and describes reasonably well many properties of ionic solutions. However, it cannot describe all experimental properties just reflecting its limitations. However, simple models can be useful to learn some physics, and here we shall illustrate that with three examples: the solvation of water around a planar ion [6] (nitrate), the impact of complex formation on the viscosity [7] for a transition metal (ferrous cation) and some simple ideas about how to distinguish between ions that are considered as structure breakers from those ions that are considered as structure makers [8].

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Devitrification and melting in vapor deposited ice

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The equilibration dynamics of ultrastable glasses under heating protocols has recently attracted significant experimental and theoretical interest. Using molecular simulations of the monatomic water (mW) model, we investigate the devitrification and "melting" behavior of both conventional annealed or quenched (QG) and vapor deposited (DG) amorphous ices subjected to controlled heating ramps [1]. By developing an algorithm to reconstruct hydrogen-bond networks, we show that bond ring statistics correlate with the structural stability of the glasses (see Fig. 1) and allow tracking crystalline and liquid clusters during devitrification and melting. We find that QG melts in the bulk, whereas melting in DG preferentially initiates near the free surface (see Fig. 2). During devitrification, the DG exhibits an excess of five-membered rings near the free surface, consistent with its tendency to nucleate the crystal phase in this region. Furthermore, the DG displays an Avrami exponent exceeding the standard 1 + d scaling, while both glasses exhibit similar sub-3d growth of liquid clusters across heating rates. This indicates that the enhanced Avrami exponent in the DG originates from its higher kinetic stability rather than from differences in growth dynamics.

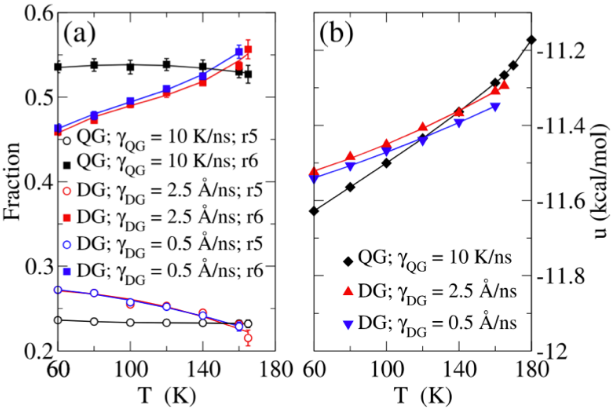

Fig. 1: (a) Fraction of rings of degree 5 (r5) and 6 (r6) vs temperature for the QG and the DG at different deposition rate γ. (b) Potential energy per particle for QG and DG.

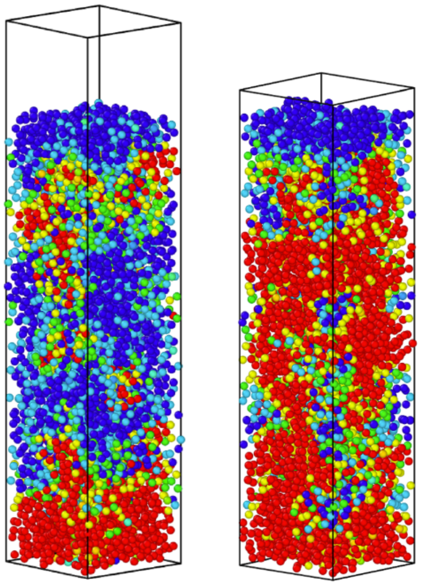

Fig. 2: melting particles in blue for the QG (left) and the DG (right) glasses.

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Observation of a mixed close-packed structure in superionic water

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In this talk we address the superionic phase of water under extreme pressure–temperature conditions. In this regime, oxygen atoms form a crystalline lattice while hydrogen ions remain highly mobile, producing a state that bridges solid and liquid behaviour and exhibits exceptional ionic conductivity.

Since its theoretical prediction [1], superionic water has been the subject of intense investigation, yet key questions persist regarding its melting curve and the stability of competing oxygen sub-lattices. Experimental studies in diamond anvil cells (DACs) have yielded conflicting results [2], while data at higher pressures obtained using dynamic compression techniques remain both scarce and inconsistent [3], reflecting the considerable experimental challenges.

Here, we present ultrafast X-ray diffraction measurements of water dynamically compressed by multiple shock waves, performed at state-of-the-art X-ray free-electron laser (XFEL) facilities. These experiments reach pressures up to 200 GPa and temperatures of 2000–3000 K, providing new constraints on the debated region of the water phase diagram encompassing the superionic phase. In particular, within 148(10)–180(20) GPa and 2445(150)–2700(350) K, we identify a mixed close-packed oxygen lattice, offering experimental support for the complex phase behaviour predicted by recent *ab initio* calculations [4].

The structural sensitivity achieved under these extreme conditions represents a significant step forward, enabling improved characterisation of the oxygen lattice and revealing associated defects. Altogether, these results open new perspectives on the physics of superionic ice, with important implications for understanding matter at extreme conditions and for modelling the interiors of water-rich giant planets.

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Quantum-driven criticality in high-pressure ice

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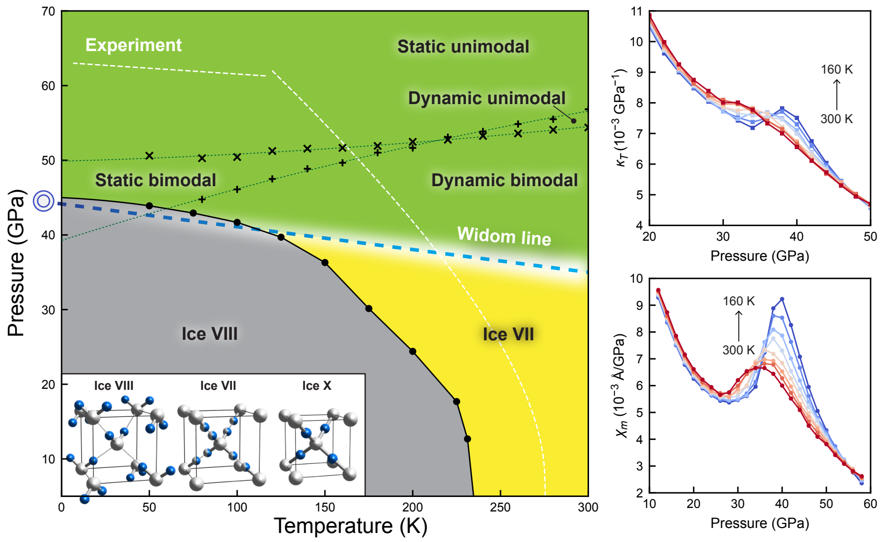
Distinct Roman numerals were once assigned to the proton-disordered molecular phase (ice VII) and the hydrogen-bond symmetrized atomic phase (ice X). However, the existence of a thermodynamic phase boundary is now heavily debated, and the microscopic origin of the seemingly continuous transformation remains unresolved. Critically, anomalous lattice softening robustly precedes this structural symmetrization. Here, utilizing path-integral molecular dynamics (PIMD) simulations with a machine-learning potential, we demonstrate that this anomalous softening originates from a Widom line emanating from a hidden critical point completely obscured by the proton-ordered ice VIII phase. This Widom line marks a criticality driven by the profound quantum delocalization of the proton sublattice. We reveal that the regime emerging above the Widom line is a quantum proton liquid, characterized by collective multi-particle tunneling constrained by the ice rules. Upon cooling, this dynamic state evolves into a quantum paraelectric ground state. Our findings reframe the continuous ice VII-to-X transformation as a manifestation of unconventional nuclear quantum criticality. Because this criticality emerges independently of a strict zero-temperature critical point defined by order-disorder suppression, it may be ubiquitous in compressed molecular solids.



Phase diagram of bcc ice polymorphs (left) alongside the critical anomalies of isothermal compressibility (top right) and local dipole susceptibility (bottom right).

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A new meta-analytical Gibbs energy equation of state for ice VII-X

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A novel hybrid equation of state (EoS) for ice VII-X has been constructed spanning from 0 to 450 GPa and 0 to 2,000 K. It combines high-accuracy low-pressure experimental volume data with vibrational energies and heat capacities derived from ab-initio computational densities of state [1] within a Mie-Grüneisen framework [2]. Most previous attempts to construct equations of state for ice VII-X have relied solely on a single data source, and while these approaches have yielded valuable insights within specific P-T regimes, they fall short in terms of generality and accuracy in extrapolated regions. To date, no unified EoS has been developed that encompasses the entire P-T range of existing measurements, while simultaneously integrating all available datasets. This hybrid methodology is aligned with state-of-the-art strategies employed in generalized EoS formulations established by renowned organizations like NIST and the IAPWS.

The EoS is implemented using a flexible local basis function representation [3], allowing most data to be fit within uncertainties; This also facilitates the use of a 0 K Helmholtz energy representation for the cold compression curve, the spline knot multiplicity of which is informed by the locations of higher order transitions [4]. As part of the open-source SeaFreeze software [2], the EoS allows for the self-consistent determination of thermodynamic properties such as density, heat capacity, compressibilities, thermal expansivity, sound speed, and phase boundaries through computationally efficient numerical evaluation.

In total, more than 1,000 measurements are considered and compared, including those delineating phase boundaries with liquid water and ice VI (the VI-liquid-VII triple point is determined as 2.101 GPa and 350.9 K). We resolve several signatures of the second order transition to ice X, including in the specific heat representation and the volume dependence of the thermodynamic Grüneisen parameter. Literature phase transition data are reproduced to within 4%, and a larger slope for the VI-VII transition is resolved than in previous experimental and computational studies [5, 6] (Fig. 1). Volume residuals remain within 5% for experimental measurements, and within 15% across the entire domain (Fig. 2).

The hydrosphere structures of large water rich exoplanets are largely controlled by the high-pressure low-temperature phase diagram of water, especially in the domain of ice VII-X. Therefore, the EoS can be used to derive new mass-radius relations of large water-rich exoplanets with improved accuracy and has implications for the potential habitability of deep exoplanetary hydrospheres [7].

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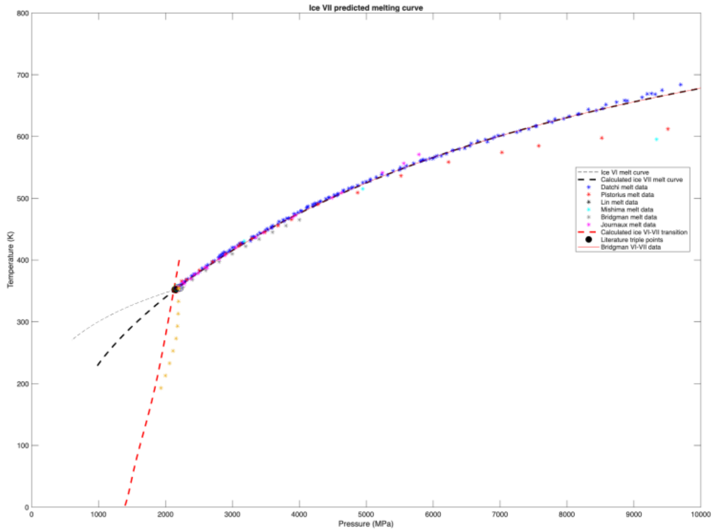

Fig 1: Predicted melting curve for ice VII and VI-VII transition compared to literature data.

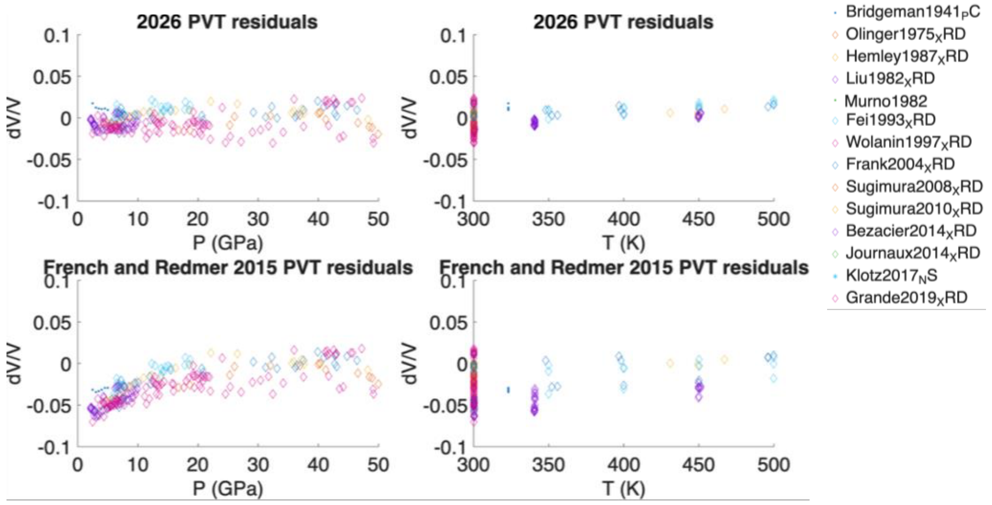

Fig 2: Volume residuals with respect to pressure and temperature for this representation and [6].

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Intermediate H-ordered state between ice V-XIII pair

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One uniqueness of water ice is its tremendous structural variety that originates from both sublattices of O- and H-atoms. The H-sublattice, corresponding to molecular orientations and dipoles, is the key ingredient enriching ice polymorphism. However, understanding the transitions between hydrogen order and disorder is often difficult, especially about the partially-ordered forms [1,2], because of the problem of kinetic freezing [3].

Ice V is a disordered high-pressure phase stable at 0.3‐0.6 GPa below 270 K. This phase takes at least two pathways of hydrogen ordering at 105‐120 K upon cooling [4], which are not fully understood. Its ordered form is known as ice XIII, but it is unclear where the second pathway leads to. Here, we re-examine the hydrogen-ordering process at ambient pressure using differential scanning calorimetry (DSC) [5]. Based on the time evolution of H-order under isothermal conditions, we simultaneously extract thermodynamic and kinetic information. These trends imply a different (but unknown) ordered state with boundaries at 112‐113 K and 120 K, which may also differ from both ices V and XIII in an H-order manner. Further details will be discussed in the presentation with comprehensive observations.

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Interfacial acid-base chemistry of hexylamine and nitric acid

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Multiphase chemistry at the air interface of atmospheric particles and ground surfaces impacts cloud formation, atmospheric chemistry, and human health [1]. Many of these chemical reactions are affected by acidity [2]. Using X-ray excited electron spectroscopy at near ambient pressure, we have suggested that the dissociation of acids adsorbed to ice is governed by the availability and mobility of water molecules to stabilize the dissociated ions and that the degree of dissociation at the air-ice interface differs from that predicted based on dissociation behavior in aqueous bulk solutions [3,4,5,6]. Ice and snow host chemistry relevant to the atmosphere and essential in cold regions of the Earth.

Here, we present new results of fundamental experimental work on the structure of the hydrogen bonding network of interfacial water and the dissociation of the acidic trace gas nitric acid and protonation of the basic trace gas hexylamine upon adsorption. We show results from a wide temperature range of the acid-base interfacial chemistry at -50°C and -20°C, addressing the impact of the increased liquid-like character of ice at the air-ice interface at temperatures approaching the melting point. This increased flexibility of water molecules at the air-ice interface has also been called the pre-melting or quasi-liquid layer [3]. Taken together, the data indicate a dominating role of the water availability on dissociation rather than the acidic strength or its temperature trend. We discuss how the limited availability of water may also be applied to other interfaces to explain the dissociation of acidic adsorbates there

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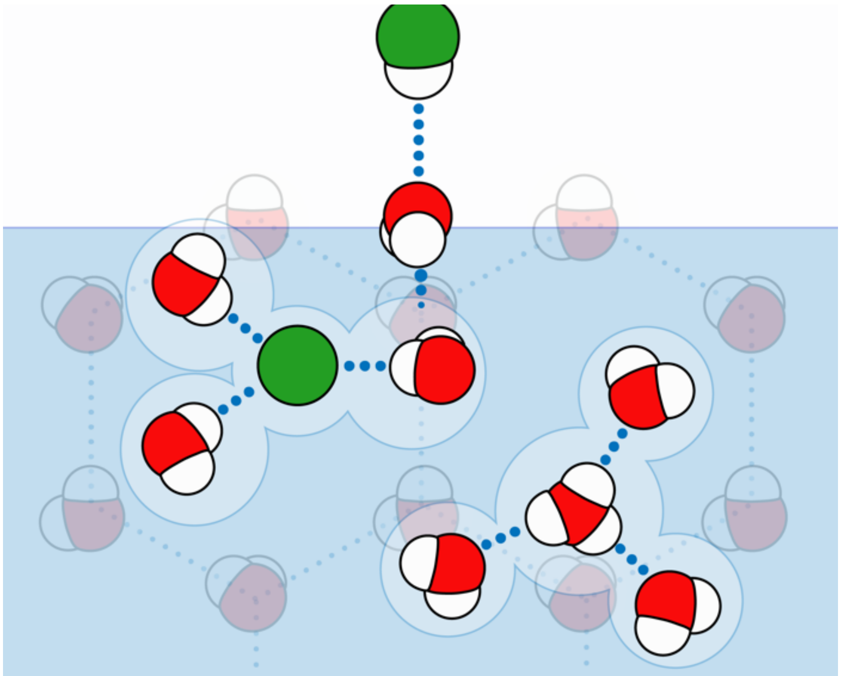

The emerging picture of acid-base chemistry at the air ice interface with HCl adsorbing at the surface and dissociating upon formation of solvation shells within the interfacial region.

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Interfacial and Confined Water through the Lens of Atomistic Machine Learning

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Water under nanoconfinement and at interfaces is ubiquitous across biology, geology, and emerging nanotechnologies. However, probing the molecular behavior of water in these environments remains profoundly challenging due to the delicate interplay of thermal fluctuations, confinement geometry, and surface chemistry. Atomistic Machine Learning Potentials (MLPs) have revolutionized the study of complex aqueous systems, bridging first-principles accuracy with the extensive molecular dynamics needed for predictive modeling [1]. In this talk, I will highlight how MLPs provide a powerful lens to uncover the anomalous behavior of interfacial and nanoconfined water.

First, I will present the diverse phase diagram of monolayer water under extreme 2D confinement, revealing exotic states such as hexatic and superionic phases [2]. Next, transitioning to solid-liquid interfaces, I will demonstrate how mechanical strain dynamically modulates the macroscopic wettability and contact angle of water on graphene [3]. Finally, I will address the longstanding debate on nanoscale water autodissociation, showing that reactivity in 2D slit pores and nanodroplets is governed by chemical potential [4].

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Structural Characterization and Infrared-Induced Restructuring of Amorphous Solid Water Deposited Between 10 and 90 K

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1 MONARIS « De la Molécule aux Nano-objets : Réactivité, Interactions et Spectroscopies », UMR8233, Sorbonne Université CNRS, F-75005 Paris, France

In the cold and dense regions of the interstellar medium, dust grains are coated with icy mantles in which water plays a key role. Amorphous solid water (ASW) is the dominant form of solid material present in these environments. Its structure, optical properties, and porosity strongly depend on deposition conditions and temperature. Recent observations by Noble et al. [1] revealed spectral features at 2.7 µm in the Chameleon I cloud that are attributed to dangling OH (dH) modes of water ice, confirming the presence of weakly bonded ice structures. Precise characterization of laboratory-grown ASW films is therefore essential as a preliminary step for studying interstellar ice analogues. To address this need, we developed the COSPINU2 device, designed to determine the optical constants of amorphous solid water deposited under ultra-low pressure at temperatures between 10 and 90 K. Our objective is to investigate the reorganization of ice under infrared irradiation using a powerful continuous-wave (CW) laser, and to compare these effects with those induced by short pulsed lasers [2–4]. This approach also aims to shed light on the quantum states of H_2 molecules adsorbed on icy surfaces.

We present the capabilities of the COSPINU2 setup to determine the thickness, density, and topology of ASW films grown between 10 and 90 K under background pressures ranging from 10^{-6} to 10^{-4} Pa. Using a dual-angle interference method, we extract the optical refractive index at 632 nm for ASW deposited at different temperatures and deposition rates. Film thicknesses, reaching up to 5 µm, are subsequently determined from near-infrared interference fringes, enabling reliable thickness calibration under each deposition condition. Localized interference patterns observed using the monochromatic green line of a low-pressure mercury lamp allow reconstruction of the three-dimensional surface topology. Our results show that at 10 K, porous ASW is metastable and undergoes sudden restructuring during growth, leading to an inhomogeneous amorphous solid composed of both porous and compact ice regions.

Spectral signatures in the mid-infrared region provide additional insight into the structural organization of the ice. Current experiments focus on water ice deposited at 25 K. Several surface vibrational modes of water ice—namely the double dangling OH (2.68 µm), triple dangling OH (2.70 µm), dangling O (2.81 µm), and s4 mode (2.85 µm)—were selectively irradiated, either individually or sequentially. Hole-burning effects and structural reorganization of the ice were observed, with additional experiments performed as a function of irradiation time. Complementary studies were conducted by varying the substrate temperature from 10 to 90 K to investigate the effects of thermal annealing. A decrease in the intensity of dangling modes and a redshift of the bulk OH stretching band were observed.

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Ice Nucleation on Disorder Surfaces – a Minimalist Model for Atmospheric Science

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Despite decades of work, predicting ice nucleation rates on realistic heterogeneous surfaces remains an unsolved challenge. In particular, atmospheric ice nucleation remains unresolved from atomistic and thermodynamic principles due to the enormous structural and chemical diversity (and complexity) of atmospheric particles. As a result, empirically fitted parametrisations remain the standard tool to describe ice formation in clouds in weather modelling.

In atmospheric science, heterogeneous ice nucleation is commonly described using the abstract concept of “**active sites”** on ice-nucleating particles, [1-3] which trigger freezing with different efficiencies. While this framework is phenomenologically successful, the microscopic origin of such sites and their connection to interfacial thermodynamics remain unclear.

To explore this connection and bridge the gap, we introduce a minimalistic toy model for heterogeneous nucleation on disordered surfaces. In this model, surface disorder is represented as a Gaussian random field describing spatial variations in interfacial free energy. Within a classical nucleation theory framework, this generates a spatial distribution of nucleation barriers, such that freezing is governed by rare favourable regions.

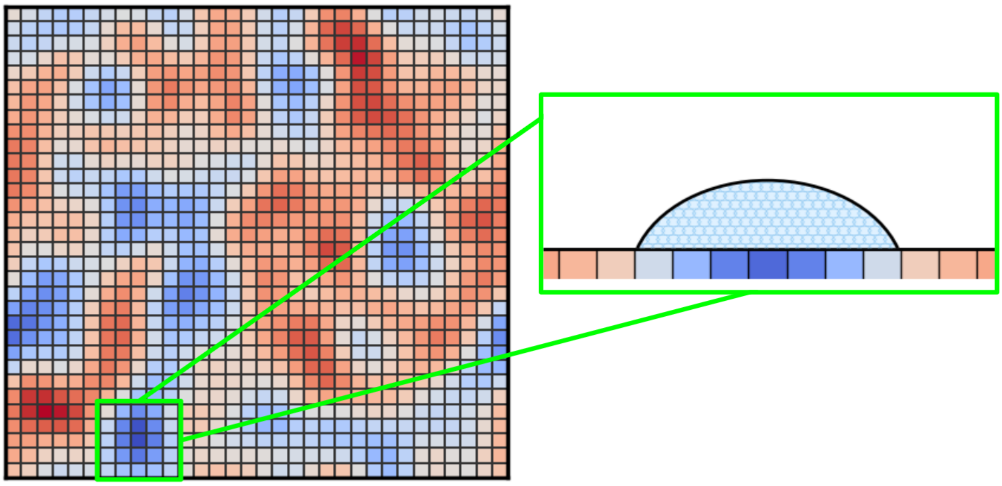

Figure 1 Schematic of the toy model. The left square represents a randomly sampled of interfacial free energy differences. “Bluer” lattice points correspond to regions where an ice interface is favorable over water. The green highlighted box highlights a region corresponding to a strong ice nucleation site

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This framework provides a simple statistical description of **chance nucleation**,[4] which has been proposed to explain the freezing of highly purified water where nucleation arises from extremely rare sites in remnant contaminants. By reducing complex surface chemistry to a small number of statistical parameters, the model offers a tractable bridge between molecular descriptions of nucleation and phenomenological representations used in atmospheric science.

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Role of lattice mismatch and substrate–water interactions in heterogeneous ice nucleation: a molecular simulation study

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Ice formation overwhelmingly occurs via heterogeneous nucleation on solid substrates. These substrates range from mineral dust to soot or bacteria, and they often possess complex structures. The relationship between their structure, their interactions with water, and their ability to nucleate ice is still not clearly understood. Here, we use molecular simulations to investigate how the structure and interactions of generic model substrates affect their efficiency in nucleating ice. To properly quantify the effects of ice–substrate lattice mismatch and the weakening of substrate–water hydrogen bonds, we study heterogeneous nucleation on substrates generated through controlled perturbations of a perfect ice lattice [1]. This approach enables us to systematically quantify the effects of lattice mismatch and hydrogen-bond weakening on heterogeneous ice nucleation. We compare results obtained using both coarse-grained (mW) and atomistic (TIP4P/Ice) water models. In addition, we consider generic substrates with simple lattice structures, such as fcc, sc, and bcc, to further explore the influence of substrate structure on heterogeneous ice nucleation [2]. Moreover, we propose an approach to obtain critical nuclei contact angles (see Fig. 1) by comparing homogeneous and heterogeneous nucleation rates under the framework of Classical Nucleation Theory [1,2].

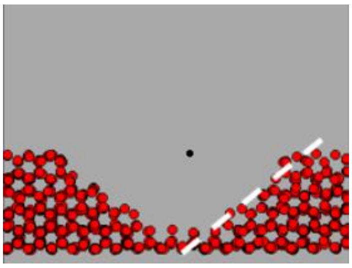

Figure 1 Ice nucleus emerged on a substrate.

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Poster Session

Molecular dynamics simulations insights into CO_2 hydrate phase diagram: beyond the traditional coexistence technique.

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Carbon dioxide (CO_2) hydrates hold promising applications in capturing and separating CO_2 for climate change mitigation [1]. Understanding their behavior at the molecular level is therefore essential, and computer simulations have become powerful tools for exploring their formation and stability, providing valuable insights into their underlying mechanisms. In this work, we perform molecular dynamics simulations to compute the three-phase coexistence line involving the stability region where CO_2 is in the vapor phase: CO_2 hydrate – liquid water – vapor. This computation was previously inaccessible using the traditional three-phase direct coexistence technique. To achieve this, we employ a novel solubility-based method [2,3], which allows us to accurately evaluate the coexistence line. Our results exhibit excellent agreement with experimental data and, for the first time, accurately reproduce the hydrate–liquid–vapor equilibrium line of the CO_2–water phase diagram. Finally, we have determined the upper quadruple point (Q_2) where the four phases, namely hydrate, liquid water, liquid CO_2, and vapor, coexist. Our pioneering result for the Q_2 value shows remarkable agreement with experimental observations, validating the accuracy of our findings and representing a significant milestone in the field of gas hydrate research.

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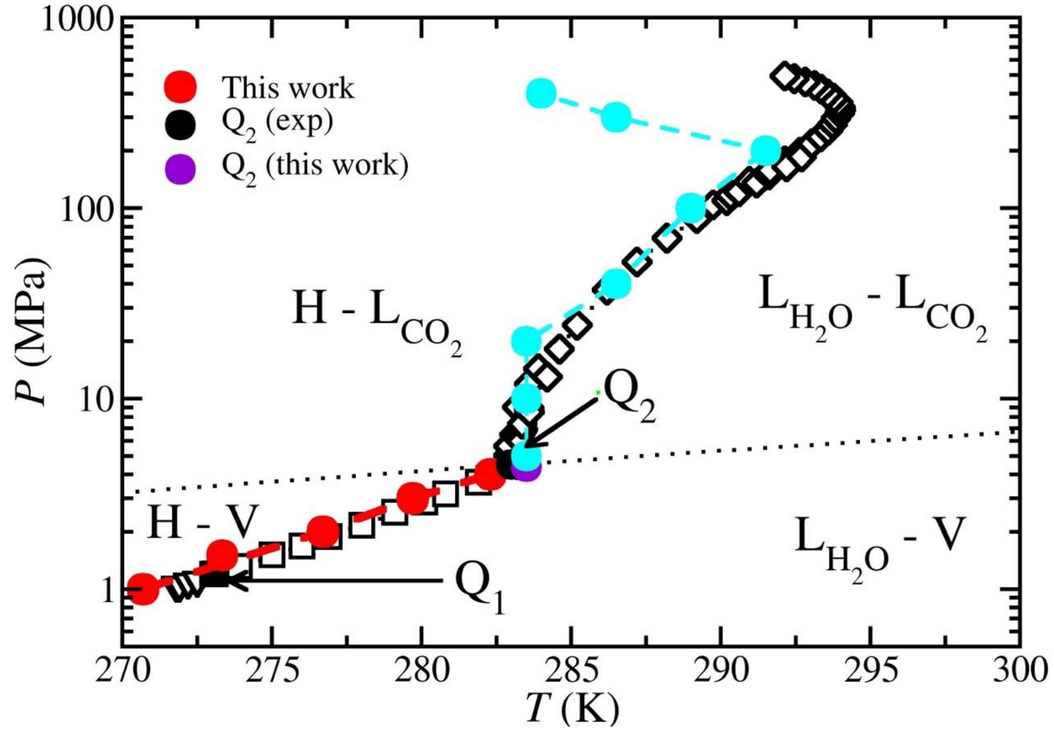

Phase diagram of the CO_2 + water mixture assuming an excess of CO_2. All black symbols correspond to experimental data taken from the literature [1]. The dotted black line represents the border between the hydrate (H) – aqueous (L_{H_2O}) – liquid CO_2 (L_{CO_2}) phase equilibria and the hydrate (H) – aqueous (L_{H_2O}) – vapor (V) phase equilibria. Cyan-filled circles correspond to simulation results obtained by some of us in a previous work [4] for the H-L_{H_2O}-L_{CO_2} three-phase line. Red-filled circles correspond to the three-phase line for the H-L_{H_2O}-V equilibrium obtained in this work. The filled violet and black circle are the simulation quadruple point Q_2 obtained in this work and the experimental point [1].

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On the importance of the dielectric constant in water modelling

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Efficient large-scale computer simulations of aqueous solutions require the use of accurate but simple empirical force fields for water. However, the complexity of these systems evidences the difficulties in describing solution properties without due account of polarization. Different strategies to remedy this problem are parameterizing water force fields to the dielectric constant or charge scaling of solvated ions.

We compare results from TIP4P/ε [1] and OPC [2] models which are parameterized to predict the dielectric constant, with results from TIP4P/2005 [3]. Our results show that TIP4P/ε and TIP4P/2005 perform equally good, with the OPC model lying significantly behind. TIP4P/ε can predict bulk phase properties of both liquid water and ice polymorphs, but also surface tensions, with an accuracy very similar to TIP4P/2005, while performing very well for dielectric constants over a wide range of pressures and temperatures [4].

The accurate prediction of dielectric constants allows TIP4P/ε to describe solution densities for model ions targeted to their crystal and melt properties, such as Joung-Cheatham model. This is achieved without the need to rescale charges, modify the Lorentz-Berthelot rule or tune the ion's Lennard-Jones parameters.

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A Hydrogen-Bond Connectivity Descriptor Based on Graph Theory

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Hydrogen bonds play a central role in determining the structure and behaviour of liquids, particularly water, the anomalous properties of which arise from its extended and highly heterogeneous hydrogen-bond network. Here we introduce a graph-theoretical framework related to the Node Total Communicability (NTC) that enables a systematic, molecule-resolved description of hydrogen-bond networks from Molecular Dynamics (MD) simulations [1] (see Figure 1). In contrast to our earlier related approaches with the NTC [2-4], the hydrogen-bond network is explicitly mapped onto a directed graph, allowing the asymmetric nature of hydrogen bonding to be retained. The method captures both local and longer-range connectivity, providing a unified metric to probe structural organization of molecules. As a representative test case, we apply this approach to water and aqueous salt solutions, demonstrating how the presence of ions modifies hydrogen-bond connectivity. From this perspective, the analysis shows that ionic effects are confined to the first hydration shell, while the hydrogen-bond network beyond remains essentially unperturbed.

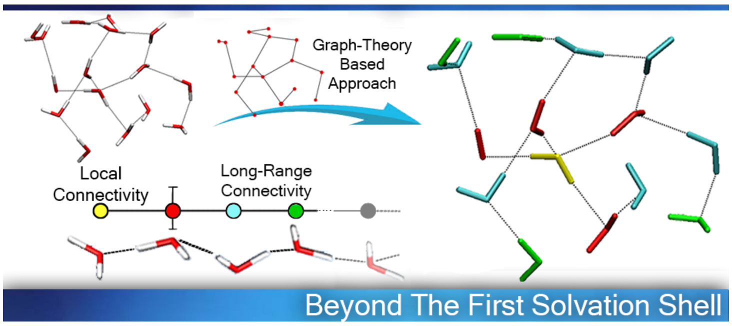

Figure 1: Schematic representation of the Graph-Theory approach developed to characterize hydrogen bond networks

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Theoretical description on high-order harmonic generation in liquid water

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High-order harmonic generation (HHG) is a highly non-linear strong-field process that produces coherent extreme ultraviolet (XUV) radiation and enables attosecond spectroscopy of ultrafast electronic dynamics [1]. Its investigation in liquids remains limited due to experimental challenges, despite the central role of liquids in chemistry and biology. The first experimental demonstration of HHG in liquids in 2018 [2] opened a new field in which many fundamental mechanisms are still poorly understood.

In this work, we address this gap through two complementary approaches. First, we develop an efficient fully quantum 1D model tailored to capture strong-field electron dynamics in liquid water. Second, we perform ab initio Ehrenfest molecular dynamics simulations with the deMon2k code [3] to incorporate coupled electron–nuclear motion and realistic liquid-phase fluctuations. Together, these methods provide a robust framework for elucidating the microscopic origins of HHG in liquid water and guiding future theoretical and experimental developments.

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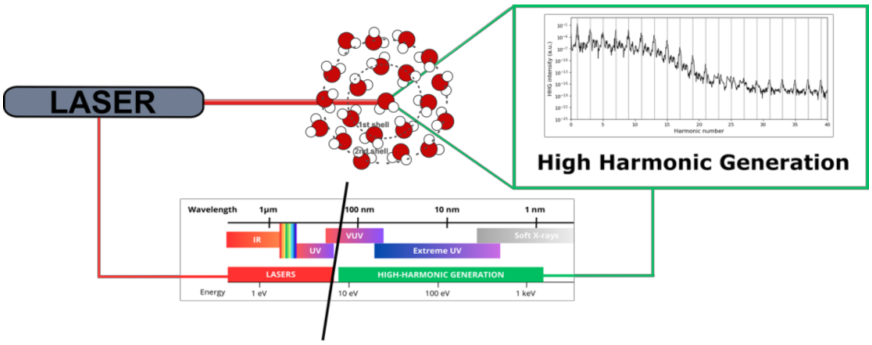

Schematic illustration of strong-field laser interaction with liquid-phase water and the resulting high-order harmonic emission.

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Dynamics of Coalescence in Hyperquenched Glassy Water Probed with Coherent X-rays

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We investigate the dynamics, morphology and structure of a deposit of thousands of micrometer-sized glassy water droplets, known as hyperquenched glassy water (HGW) [1]. This type of glassy water is relevant to cryochemical techniques, especially cryo electron microscopy (cryoEM) [2] or synthesis of 'unstable' intermediates, such as carbonic acid [3]. We previously reported droplet coalescence of HGW starting from ~125 K upon heating [4] and now focus on the structural nanoscale dynamics during and after coalescence, probed using X-ray photon correlation spectroscopy (XPCS). During coalescence, we find an irreversible ballistic process in the temperature range 130–145 K with velocities around 0.1 to 0.2 Ås^{-1}. Additionally, if the sample is not annealed below 125 K, we observe a q-independent mode that we link to the coalescence process. After coalescence finishes, we find a sharp jump in diffusivity to approximately ~2 Å^{2}s^{-1} at about 148 K, revealing significant diffusive dynamics. From these results, we conclude that the coalescence process is driven by ballistic, non-diffusional dynamics below roughly 136 K, while nanoscale diffusion is observed above. We link the jump in diffusivity after coalescence to the glass transition in HGW. [5]

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Methane Hydrate Growth Kinetics in Swelling Clays Controlled by Interlayer Water

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Natural gas hydrates (NGHs), predominantly composed of methane, constitute a major carbon reservoir in the world and play an important role at the intersection of water, energy, and geosystems [1]. However, hydrate formation and distribution in clay-rich environments remain poorly constrained, despite their critical implications for methane release, sediment stability, and subsurface fluid storage. Smectite clays exhibit complex swelling behavior, including extensive interlayer expansion, potentially modifying local water activity and hydrate growth pathways [2]. Field observations of anomalously low large-to-small cage occupancy ratios in smectite-rich sediments further indicate that clay-water interactions may drive non-equilibrium hydrate formation [3]. In this study, we investigated methane hydrate growth in swelling and non-swelling clay matrices using complementary neutron diffraction and Raman spectroscopy. Our results provided direct experimental evidence of hydrate formation within swelling clay systems and demonstrated that cyclic interlayer swelling and deswelling control water transport, hydrate growth kinetics, and cage occupancy. These processes make a distinct, non-equilibrium hydrate formation regime that differs fundamentally from hydrate growth in sandy or bulk-water-dominated systems. By elucidating how clay mineralogy and water activity jointly control hydrate formation and distribution, this study advances the understanding of NGHs in clay-rich sediments and offers new perspectives on hydrate-related geohazards and geological CO_2 storage in clay-rich reservoirs.

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Ab Initio speciation and spectroscopy of nitric acid solutions

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A fundamental property of nitric acid, its dissociation constant in water, is still debated by recent studies, due to speciation uncertainties in the water-nitric acid (H_2O-HNO_3) system. Notably, the existence of an ion pair (NO_3^- - H_3O^+) lay doubts about Raman determination of free nitrate concentration. In this work, we revisit the current arguments under the light of molecular-scale simulations. Using the PBE-D3 and R2SCAN functionals in the framework of density functional theory to calculate the interactions, we perform ab initio molecular dynamics of the system at different concentrations (1, 5, 9, 16, 25 and 37% mol HNO_3) at 330K. We then perform finite-field calculations on snapshots extracted from the trajectories to calculate the corresponding Raman spectra, and link them with the nature and the concentration of various species. We find that, unexpectedly, R2SCAN greatly underestimate the dissociation of nitric acid, while PBE-D3 slightly overestimate it. The AIMD Raman spectra reproduce quite well the experimental ones, with a slight red-shift of vibration. Notably, the 1046cm^{-1} experimental signal, corresponding to the nitrate asymmetric stretching of N-O bonds, is predicted near 1032cm^{-1} by PBE-D3. As hypothesized experimentally, area integration of this signal is linear with free nitrate concentration. Whether the ion pair NO_3^- -H_3O^+ is considered free nitrate or not doesn't affect significantly the resulting dissociation constant, as it affects it by approximatively the same uncertainty previous experimental studies concluded on.

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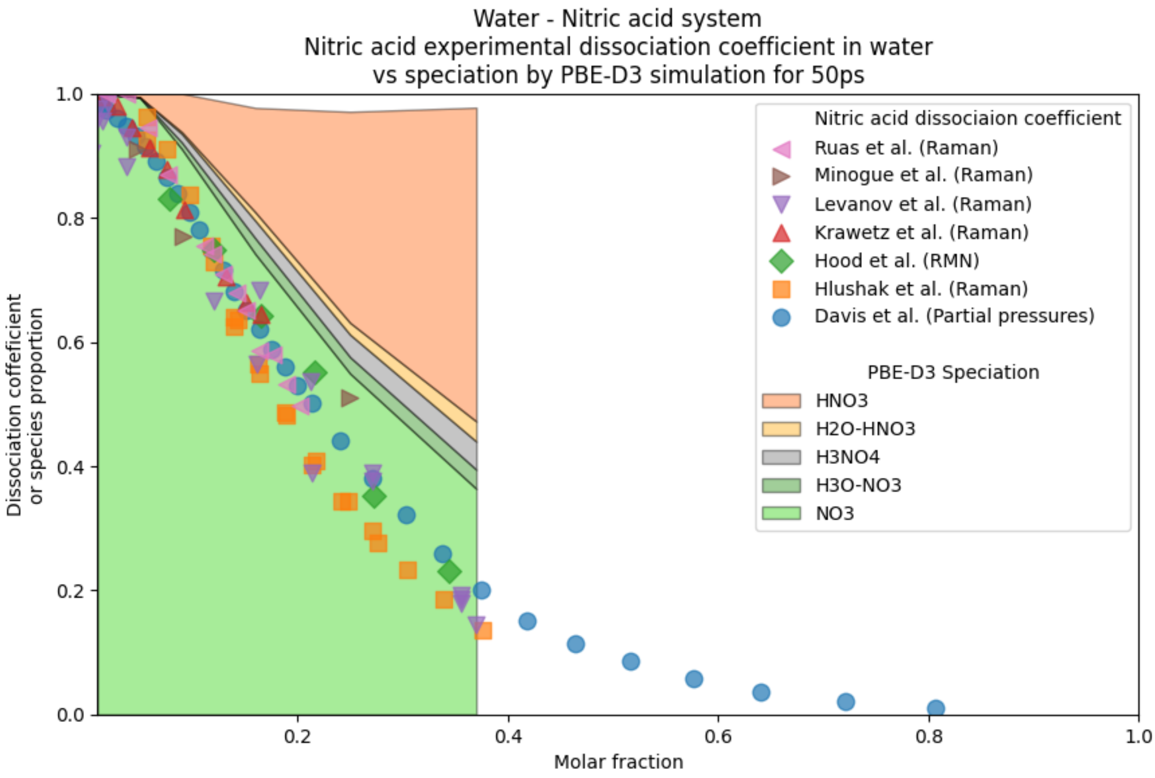

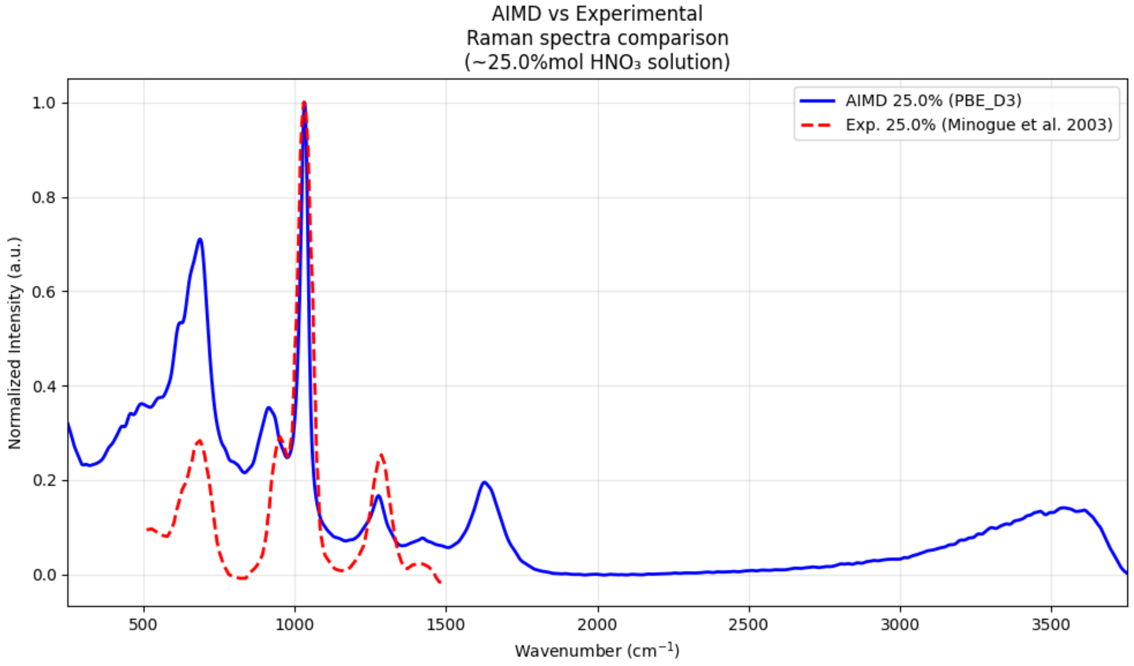

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Water intrusion/extrusion in MOF and energy absorption.

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A key aspect of energy storage in nanoporous materials is the intrusion of water into their pores, a process that converts mechanical energy into interfacial energy. This phenomenon depends on the pore size but essentially on the chemical nature of the material surface, ranging from hydrophilic to hydrophobic. The intrusion requires the application of external pressure governed by the Laplace law. The intrusion/extrusion processes and their implications for energy storage are studied thanks to the combination of homemade high-pressure calorimeter and high-pressure neutron diffraction experiments performed at the LLB and the ILL. With a special focus on MOF materials, such as Zif-8 (zeolitic imidazolate framework), we compare under quasi-static loading conditions the amount of energy implied and the amount of water intruded by numerical calculations, associated to a reversible material deformation. Interestingly, while confinement is known to enhance the differences in behavior between H_2O and D_2O, this difference is even more pronounced in the intrusion/extrusion processes.

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NaCl-Bearing Salty Ice VII with Implications for Modelling of Icy Moons

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The interiors of icy bodies in the outer Solar System are commonly modelled as being composed predominantly of pure water-ice phases. The detection of NaCl-rich ice grains in the plumes of Enceladus, the presence of salt components in Saturn's rings and the remote spectroscopic observations of salt on the surfaces of Europa and Ganymede all indicate that the H_2O-NaCl system is relevant to planetary interiors [1-3]. Here, we report on the previously unknown NaCl-bearing salty ice VII phase formed at thermodynamic conditions relevant for these planetary bodies. Using synchrotron X-ray and neutron diffraction techniques, we show that this phase exhibits a markedly expanded lattice with a unit cell volume approximately 7-10% larger than that of pure ice VII. Measurements under decompression reveal that the phase is unstable below ~5GPa, decomposing into pure ice VII and crystalline NaCl. We determine its isothermal equation of state up to 40 GPa, which is well described by a modified third-order Birch-Murnaghan [4] equation of state. These results demonstrate that NaCl can incorporated into the ice VII structure and affects density and physical properties of high-pressure ice, with important implications for the internal layers distribution of icy planetary interiors.

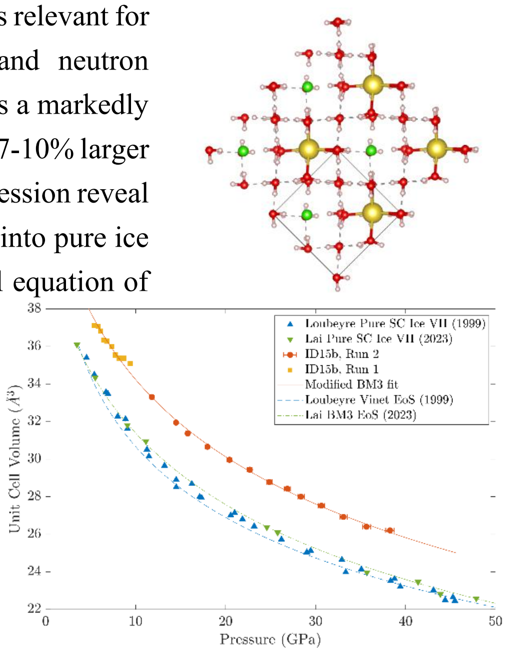

Fig.1 – Structure and Equation of State for NaCl-bearing ice VII

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Applications of high-pressure water phases to interior structure models of large Icy moons

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Ganymede is the largest moon in the Solar System and possesses an extensive hydrosphere, including a possible subsurface ocean beneath its outer ice-I shell [1, 2]. Its low moment of inertia factor [3] ,together with the presence of an intrinsic magnetic field [4], indicates that Ganymede is fully differentiated and likely hosts a liquid metallic core and an extensive high-pressure ice layer, potentially composed of multiple ice phases (Fig. 1), between the ocean and silicate mantle. Similarly, Callisto and Titan could also harbor interesting and exotic hydrosphere structures [5, 6].

In the context of the upcoming exploration of these moons by JUICE and Dragonfly, we have developed new models of their interior structure and computed their expected surface heat flux, magnetic induction response (Fig. 2), tidal deformation (Love numbers) and tidal dissipation. The hydrosphere is modeled using equations of state of pure water ices and NaCl aqueous solutions with varying concentrations, following the SeaFreeze formulation [7]. Convection in the ice-I shell is modeled with scaling laws derived in [8]. Measurements of moment of inertia and magnetic induction, together with estimates of the available heat sources, are used to determine the possible present-day hydrosphere structures of large icy moons.

An analysis of the computed tidal Love numbers and magnetic induction response allows us to determine which hydrosphere properties can be constrained by the expected future measurements of JUICE and Dragonfly. These models would significantly benefit from laboratory measurements of the mechanical, thermodynamic, and electrical properties of water–ice mixtures containing different salts at pressures from 0 to 2 GPa and temperatures from 220 to 320 K.

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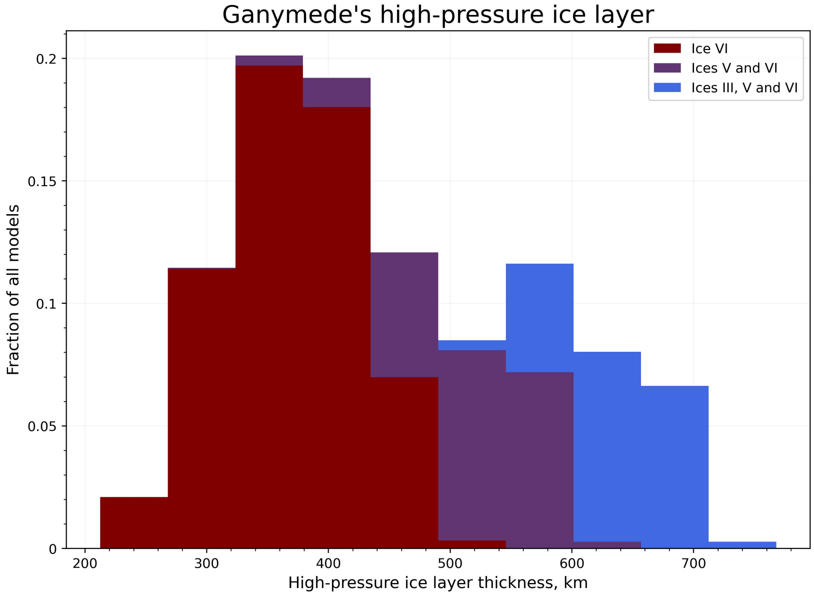

Fig. 1.
Histogram showing the distribution of the total thickness of the high-pressure ice layer for acceptable Ganymede interior models and the associated ice phases.

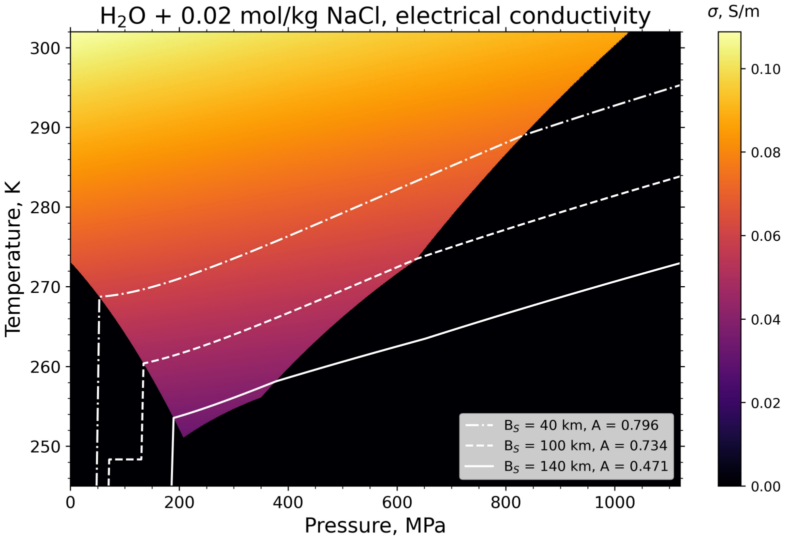

Fig 2.
Three models of Ganymede's hydrosphere shown on water's phase diagram. The liquid phase contains 0.02 mol/kg of NaCl, and for each model the magnetic induction efficiency A is indicated in the legend. The electrical conductivity of the brine was computed following Psarakis et al. 2024.

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How Water Dictates the Structure of Liquid and Amorphous Ammonia Dihydrate

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The complex phase diagram and polyamorphism of pure water remain among the most debated topics in condensed matter physics. However, the structural behaviour of water within binary mixtures, where the hydrogen-bond network is perturbed by co-solvents, offers a unique lens through which to understand these phenomena. We present a comprehensive structural investigation of Ammonia Dihydrate (ADH), a key chemical constituent of icy planetary bodies, across its liquid and amorphous solid states.

Using high-resolution neutron diffraction coupled with Empirical Potential Structure Refinement (EPSR) and DFT-based modelling, we characterize the local and intermediate-range order of ADH. We demonstrate that flash-freezing ADH at 100 K yields an amorphous solid that is structurally distinct from its parent liquid, characterized by a narrower but larger water-water coordination and shift in the distribution of hydrogen-bonded rings.

We identify a pressure-induced structural crossover characterised by the collapse of the second coordination shells. Simultaneously, the hydrogen-bond network topology reorganises via a fragmentation stage shifting from five-membered to four-membered ring dominance. These findings suggest that ammonia stabilizes a unique hybrid state maintaining the local tetrahedrality of low-density amorphous ice while adopting the efficient packing of high-density phases. This study provides a new framework for understanding how guest molecules dictate the structural variety of water-rich networks and offers broader implications for the study of aqueous solutions under extreme conditions.

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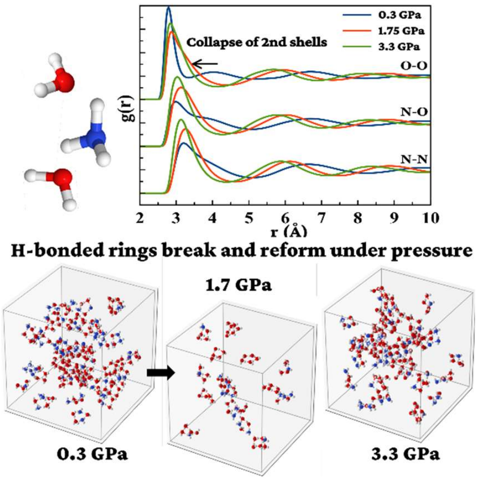

(Top) Calculated intermolecular partial g(r) for high-pressure amorphous ammonia dihydrate, showing the collapse of the 2nd coordination shells. (Bottom) Simulated boxes depicting how the hydrogen-bonded rings reorganize with pressure

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Dual quantum locking: Dynamic coupling of hydrogen and water sublattices in hydrogen filled ice

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Hydrogen hydrates, particularly the C2 phase [1], offer a unique architecture where water and hydrogen form two interpenetrating, strongly coupled crystalline networks that behave as a unified quantum system. At extreme pressures, the high-density confinement of hydrogen within the ice lattice triggers a profound entanglement: the water lattice no longer acts as a passive host but actively modifies hydrogen dynamics and amplifies its quantum effects [2]. This talk explores the pressure- and temperature-driven phase transitions within this framework, revealing how the symmetrization of hydrogen bonds in the ice is coupled to a transition to an orientational nematic phase in the hydrogen sub-lattice [3]. Using a combination of path-integral molecular dynamics (PIMD), quantum embedding, and high-pressure experiments including Raman spectroscopy and synchrotron X-ray diffraction, we demonstrate that this quantum-induced ordering occurs at significantly lower pressures than in pure hydrogen.

Our ongoing work utilizes Machine Learning Interatomic Potentials (MLIP) to extend these simulations to larger, more complex systems, facilitating deeper insights into the behavior of hydrogen-rich quantum materials. These results establish hydrogen-filled ices as unique model systems for exploring confined quantum matter, offering new perspectives for both planetary science and the design of materials for hydrogen storage.

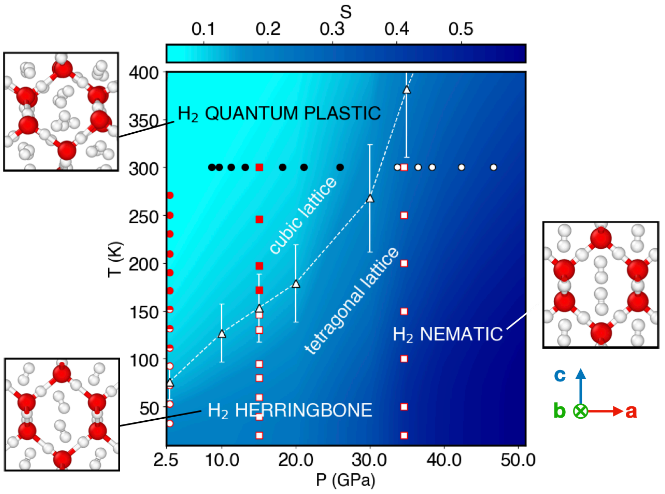

Figure 1 - Pressure-Temperature phase diagram of the C2 hydrogen hydrate, combining quantum embedded calculations and experimental data. XRD data (circles) and Raman measurements (squares) are shown, with symbols indicating cubic (filled) and tetragonal (open) phases. The background color represents the H2 orientation factor S, and white triangles with error bars correspond to simulations. Dashed lines highlight the cubic-to-tetragonal transition. Insets show DFT- optimized geometries for the quantum plastic, herringbone, and nematic phases

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Shape selection in ice: kinetic roughening versus interfacial control

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Ice crystal morphology reflects competing interfacial mechanisms that are often difficult to disentangle[1]. Here we distinguish intrinsic kinetic roughening from extrinsic interfacial control during near-equilibrium ice growth. Using cryomicroscopy and quantitative real-time image analysis, we study ice crystals grown from aqueous solutions containing non-adsorbing colligative solutes (dimethyl sulfoxide and proline) and selected salts.

We identify a sharp roughening transition at $T_R = -16.0 \pm 0.2$ °C, marking a change from rounded crystals above T_R to faceted hexagonal plates below T_R, independent of the identity of non-adsorbing solutes[2]. Roundness varies sigmoidally across T_R, consistent with a transition in growth mode, while melting remains isotropic, revealing a marked asymmetry between growth and dissolution[2]. Salts introduce distinct interfacial effects[3]. Ions excluded from the lattice modify interfacial water structure and alter anisotropic shape selection without adsorption-mediated pinning. In contrast, ions that incorporate into the lattice destabilize facets and suppress hexagonal shaping, restoring isotropic growth. Subfunctional concentrations of antifreeze protein type III induce faceting above T_R, shifting the effective threshold and confirming adsorption-mediated pinning as a separate and dominant mechanism[4]. Together, these results demonstrate that ice crystal shape emerges from competition between intrinsic roughening, lattice incorporation effects, and protein pinning, providing a unified framework for understanding symmetry breaking at the ice-liquid interface.

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Pressure-Driven Changes in Methane Hydrate II: Insights into Water–Methane Interactions in Planetary Ices

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Methane and water are among the most abundant materials in the outer solar system and play prominent roles in the internal structure of icy planets such as Titan, Neptune, and other ice-rich celestial bodies. Methane hydrate II (MH-II) is found in the icy mantle of Titan. It is speculated that methane hydrate and methane reservoirs in this region are the origin of Titan's methane-rich atmosphere [1]. A full understanding of the volatile nature of methane hydrate is important for mapping the internal structures of Titan and other icy bodies and for providing insight into water–hydrocarbon interactions under extreme conditions.

Methane hydrate II is a structural phase of methane hydrate that is stable between 1.1 and 2 GPa at room temperature. Its structure consists of a large barrel-like ice cage capable of hosting multiple guest methane molecules, and two smaller ice cage types [2]. In 2001, Shimizu et al. collected photomicrographs and neutron diffraction data on methane hydrate II [3]. From their findings, they theorised a non-structural phase transition at 1.3 GPa. Recently, a study has suggested a change in space-group at this pressure [4]. Our experiment set out to explore this behaviour using Raman spectroscopy and x-ray diffraction, which, up to that point, had not been used to characterise methane hydrate due to the low scattering nature of its atomic structure. Our findings from these experiments will be presented and discussed.

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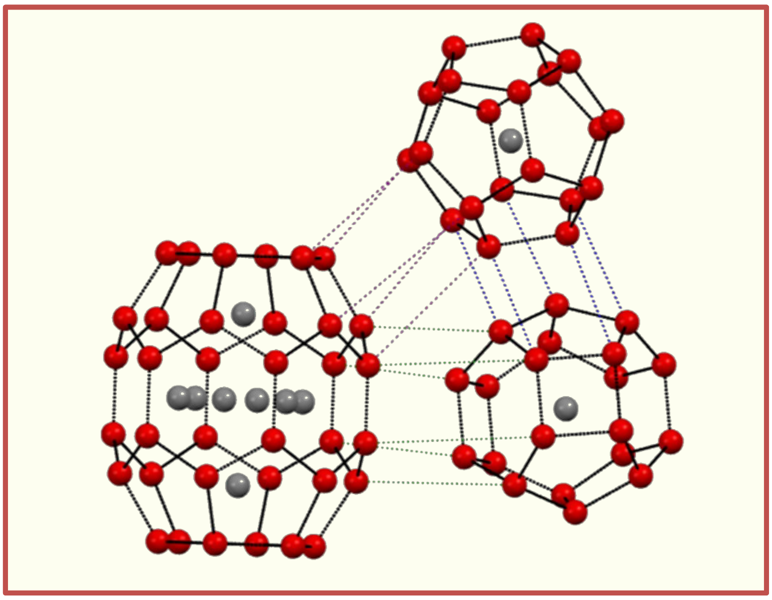

Figure1: Structure of methane hydrate II produced from data collected via x-ray diffraction at the European Synchrotron Radiation Facility (ESRF)

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Dynamical and structural properties of aqueous solutions at ambient conditions with machine learned force field.

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The dynamics of water shows anomalous, ion-specific behavior in electrolyte solutions. A paradigmatic example is the enhancement of water diffusion in CsI solutions and its slowdown in NaCl solutions relative to neat water. This anomalous diffusion is not accurately described by typical force-field–based molecular dynamics simulations due to an inadequate description of ion–water interactions.

In this work, we present a study of the anomalous diffusion of water induced by the presence of either NaCl or CsI in ionic solutions at ambient conditions by classical Molecular Dynamics simulations employing a many-body force field within the MACE Machine Learning framework [1]. The force field is trained on DFT energy, forces and stress with the revPBE-D3 [2] approximation which is considered a good compromise between accuracy and efficiency.

Our predictions of anomalous diffusion agree with experimental data both for CsI and NaCl [3] solutions and show an improvement in the description of the dynamical behavior of NaCl solutions as a function of concentration compared to previous results obtained with a different machine-learning framework (DeePMD) [4].

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Thermodynamics of Methane Hydrate Inhibition in Mixed Aqueous Systems: Experiments, Modeling, and Validation

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This work presents a comprehensive investigation of methane hydrate formation thermodynamics in aqueous solutions. Phase equilibrium (V–L_w–H) measurements were conducted for methane in systems containing monoethylene glycol (MEG), methanol (MeOH), their binary mixtures (3:1, 1:1, 1:3 mass ratios), the industrial reagent Glycoil-1, and its 1:1 mixture with MeOH. Experiments covered pressures of 3–25 MPa and inhibitor concentrations up to 60 mass%. All inhibitors shifted equilibrium to lower temperatures, with effectiveness increasing proportionally to MeOH content. A notable synergistic effect was observed: at concentrations exceeding 10 mass%, the inhibitory effect of MeOH/MEG and MeOH/Glycoil-1 mixtures exceeded the additive sum of individual components, with synergy parameters reaching 21–30% at 60 mass%.

The experimental data were validated through thermodynamic consistency checks using ice freezing point depression measurements (0.1 MPa, up to 60 mass%), which demonstrated strong linear correlations between hydrate equilibrium temperature suppression and ice melting point depression.

High-pressure visual cell studies revealed that inhibitor composition influences nucleation sites and crystal morphology. MEG promoted interfacial nucleation and exhibited anti-agglomerating properties. Complementary density and viscosity measurements (0–30 °C, atmospheric pressure) showed that MeOH dilution of MEG solutions significantly reduces viscosity while minimally affecting density. The practical relevance of mixed inhibitors was demonstrated through case studies showing that MeOH/MEG mixtures can reduce specific inhibitor consumption by half and enable lower gas separation temperatures compared to conventional MEG solutions.

This work was supported by the Russian Science Foundation (grant 25-19-00284), https://rscf.ru/project/25-19-00284/

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Advanced Laboratory Workflow for Evaluating Confined Fluids and Pore Connectivity in Bazhenov Tight Shales

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Organic-rich shales, including the Bazhenov Formation, are characterized by intricate nanoporous systems, wherein fluids are confined within highly heterogeneous pore networks. In such environment, the behavior and distribution of water remain insufficiently constrained, particularly due to strong interactions with mineral surfaces and organic matter. The present work is focused on the characterization of confined fluids, with particular attention to aqueous phases in tight shales.

An integrated experimental workflow was applied, combining low-field nuclear magnetic resonance (NMR) relaxometry, micro-computed tomography (μCT) with Xe contrast, standard petrophysical measurements, Rock-Eval pyrolysis, and sequential solvent extraction with SARA (saturates, asphaltenes, resins, aromatics) analysis. Core samples covering a range of thermal maturity were examined to evaluate fluid distribution, pore accessibility, and confinement effects.

The results reveal that NMR relaxation data can be utilized to differentiate between mobile and bound water, encompassing clay-associated and nanopore-confined fractions. A stepwise extraction procedure was conducted to investigate the effects of hydrocarbon removal on pore accessibility and fluid redistribution. μCT observations were performed to analyze the progressive development of pore connectivity and the pivotal role of organic matter in regulating fluid confinement. These findings demonstrate that the extraction process alters pore accessibility, leading to the redistribution of confined fluids.

Measured porosity increases by up to a factor of two after decane saturation, indicating that confined fluids strongly affect pore volume estimates. The proposed approach enhances the characterization of fluid distribution and facilitates the development of more realistic pore-scale models for unconventional reservoirs.

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Two molecular pathways for ion-driven “structure making / breaking” in water revealed by Correlated Vibrational Spectroscopy

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Aqueous anions are commonly classified as “structure makers” or “structure breakers” based on how they affect water, which is deduced from macroscopic observables such as the viscosity B-coefficient, yet the underlying molecular mechanisms remain debated because most spectroscopies do not directly isolate water–water hydrogen bonds. Here we use Correlated Vibrational Spectroscopy (CVS)[1], a hyper-Raman based approach that separates self-correlated (single-molecule / isotropic) from cross-correlated (collective / interacting) vibrational responses, thus isolating the cross-correlated water–water H-bond stretch near 205 cm^{-1}. Which allowed us to quantify the changes in strength of orientationally cross-correlated H-bonds (and associated charge-transfer contributions), and the number of such interacting H-bonds.

We apply CVS to 2 M sodium salt solutions spanning halides and oxyanions[2]. The data reveal two distinct pathways by which anions modify the water HB network. Soft, polarizable anions (I^-/Br^-/SCN^-) induce large red shifts (up to −62 cm^{-1} for I^-) together with strong increase in cross-correlated intensity (up to +56% interacting H-bonds), consistent with charge-transfer mediated weakening of individual H-bonds accompanied by an increased concentration of correlated water–water interactions. In contrast, hard anions (NO_3^-/ClO_4^-/F^-/SO_4^{2-}) show only small frequency shifts and modest intensity changes, consistent with predominantly electrostatic perturbations. These contrasting molecular responses are rationalized using Hard–Soft Acid–Base (HSAB) theory[3], showing that similar macroscopic trends can arise from fundamentally different microscopic mechanisms due to compensation between H-bond strength and the number of H-bonds.

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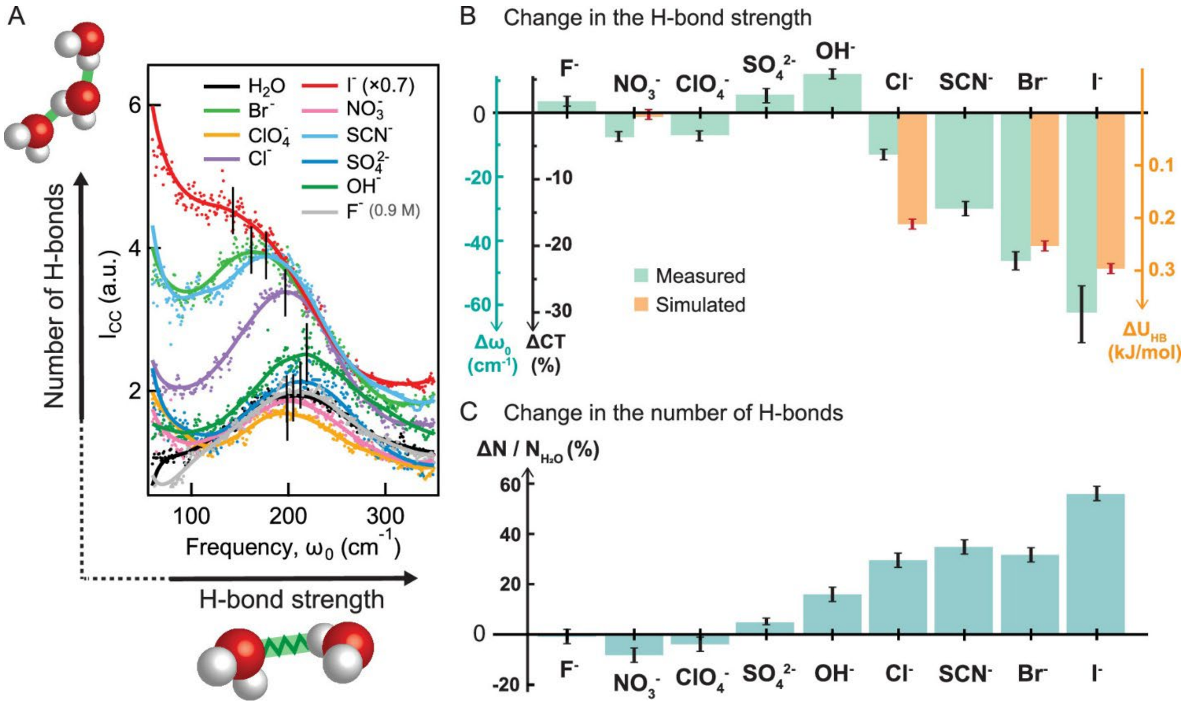

Figure 1: Ion-specific modification of the water–water H-bond network measured by CVS in concentrated sodium salt solutions. The cross-correlated H-bond stretch frequency shift reports changes in H-bond strength (and associated charge-transfer), while the intensity reports the relative change in the number of orientationally cross-correlated (interacting) H-bonds, revealing distinct behaviors for soft vs hard anions.

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WaterX - Program May 24 - May 29 2026 - La Maddalena (Italy)

time	Sunday May 24
18:30	**Welcome Cocktail**
21:00	**Opening Lecture: H. C. Allen**

time	Monday May 25
8:30	**Opening & Registration**
9:00	C. Salzmann
9:45	B. Journaux
10:15	G. Tobie
10:35	H. Kobayashi
10:55	I. Braslavsky
11:10	**Coffee Break**
11:40	F. Caupin
12:10	J. A. Troncoso
12:30	V. Molinero
12:50	F. Pabst
13:05	**Lunch**
14:30	A. Desmedt
15:00	L.-R. Fidler
15:20	L. Del Rosso
15:40	T. Poreba
16:00	K. Skrzyńska
16:15	**Excursion: Caprera Trail and beach**
19:30	**Sunset at Baia Trinita**

time	Tuesday May 26 - Chair. ....
6:00	**Sunrise Trail to Cala Napoletana #**
9:00	M. Bonn
9:45	C. Alba-Simionesco
10:15	D. Morineau
10:35	C. Vega
10:55	F. Leoni
11:10	**Coffee Break**
11:40	A. Ravasio
12:10	K. Mochizuki
12:30	U. Jones
12:45	K. Yamashita
13:00	**Lunch**
	Free Time Scuba Diving on demand **
16:00	T. Bartels-Rausch
16:30	C. Schran
17:00	X. Michaut
17:20	Z. Fakhoury
17:40	E. Sanz
18:00	**3-minute talk Poster presenters**
19:00	**Poster Session**

time	Wednesday May 27 Chair ....
9:00	H. Tanaka
9:45	F. Perakis
10:15	C. Stan
10.35	I. Saika-Voivod
10:55	R. Tyburski
11.10	**Coffee Break**
11:40	S. Xantheas
12:10	F. J. Blas
12:30	B. Chazallon
12:50	A. Stoporev
13:05	**Lunch**
14:30	N. Giovanbattista
15:00	F. Martelli
15:30	C. Pierleoni
15:50	A. Siciliano
16:05	**Coffee Break**
16:30	E. Adams
17:00	F. Turci
17:20	G. Graziano
17:40	C. Sun
18:00	I. Bako
18:20	**Walk to Punta Tegge for Sunset Apero ***

time	Thursday May 28- Chair ....
:45	K. Koga
:15	G. Franzese
:45	A. Greco
0:05	**Boat trip to Maddalena Arcipelago ##**
0:00	**Social Dinner**

time	Friday May 29 Chair ....
9:00	M. Citroni
9:30	G. Sosso
09:50	D. V. Matyushov
10:10	V. Artemov
10:30	**Coffe Break**
11:00	M. Rescigno
11:15	L. Petterson
11:30	C. Cerdeiriña
11:50	S. V. Buldyrev
12:05	**Closing**

max 10 places available.
* An apero-dinner is available at Zi’ Anto restaurant in Punta Tegge under request (price TBD).
** Scuba-diving will be operated by Best Shark Diving Center upon request (Introductory lesson and excursions available: price TBD).
This activity is NOT included in the registration fee. It should cost about € 70/person (lunch included), a local fee of 5 € will be requested when entering the Parco dell’Arcipelago.

Impact of ions on water structures and dynamics

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Ion solvation in water gives rise to strikingly ion-specific and complex behavior, but its underlying physical mechanisms remain incompletely understood, despite its central importance in nature, science, and technology. Here, we propose that the dynamic effect of solvation arises from geometrical and entropic frustration within the hydration shell. Using the non-polarizable force field for aqueous salt solutions developed by Vega and co-workers, based on TIP4P/2005 water, we systematically vary the ion–first-shell water distance, d, and ionic charge, q, revealing how ions induce a hierarchy of dipolar, translational, and bond-orientational ordering in the water molecules surrounding the ion. This ordering reflects competition between ion–water electrostatics and inter-water hydrogen bonding, quantified by a characteristic length scale, $\lambda_{\mathrm{HB}}(q)$ [1].

For certain ion sizes and charges, hydration-shell waters experience a Thomson-like geometrical constraint: arranging water dipoles on a spherical shell can either stabilize or frustrate bond-orientational order, depending on shell occupancy, angular order, and hydrogen-bond topology. Remarkably, water residence times obey a Rosenfeld-like scaling with the bond-orientational entropy of the hydration shell, indicating that hydration dynamics are governed by the loss of configurational freedom associated with bond-orientational ordering [1]. Small changes in ion parameters can therefore produce dramatic changes in hydration-shell lifetime, spanning up to eleven orders of magnitude for main-group ions. These findings identify hydration-shell bond-orientational ordering as the microscopic origin of ion-specific solvation dynamics and establish it as a guiding principle for electrolyte design. Time permitting, I will also discuss how ion-specific hydration influences the collective dynamics and transport properties of salt solutions.

Acknowledgements: We gratefully acknowledge our long-standing collaboration with Rui Shi and members of his group, which has been central to this work. We also thank Anthony Cooper for a pleasant and productive collaboration. This work was partially supported by Specially Promoted Research (Grant No. JP20H05619) from the Japan Society for the Promotion of Science (JSPS).

[1] R. Shi, A. J. Cooper, and H. Tanaka, Nat. Commun. 14, 4616 (2023).

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Density fluctuations and anomalous transport in supercooled aqueous solutions

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We investigate how nanoscale fluctuations of water control molecular transport in supercooled aqueous systems by combining femtosecond X-ray scattering with molecular dynamics simulations. Measurements on rapidly cooled glycerol–water microdroplets reveal a strong increase in isothermal compressibility upon cooling, indicating enhanced density fluctuations that persist even in dilute solutions [1].

X-ray Photon Correlation Spectroscopy (XPCS) measurements of protein diffusion show pronounced deviations from the Stokes–Einstein relation below ~230 K, with diffusion enhanced by up to a factor of ~3 [2]. A minimal two-state Langevin model, with stochastic switching between low- and high-friction environments, captures this behavior and links the observed transport anomalies to intermittent dynamics in a fluctuating medium [3].

These results establish a direct connection between water's density fluctuations and nanoscale transport in supercooled solutions.

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The impact of drop freezing dynamics on the accuracy of experiments with evaporatively supercooled water drops

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Experiments that probe supercooled water drops with X-ray free-electron lasers (XFEL) extended the investigations of supercooled water to lower temperatures and reported anomalous maxima in thermodynamic properties [1,2]. However, some of these results are inconsistent with previous data on supercooled water, such as an unexpectedly low ice nucleation rate [3]. We have recently determined ice nucleation rate using an XFEL experiment, and found it to be consistent with previous measurements [4], which suggests that earlier XFEL results had systematic errors. While it was argued that early XFEL studies underestimated the temperature [5], this is not sufficient to understand possible errors. To reach the lowest possible liquid temperatures, XFEL studies work with a mix of liquid and frozen drops, and the dynamics of freezing can affect measurements in counterintuitive ways. We have developed quantitative models of freezing in supercooled water drops [4], and of drop self-propulsion during freezing [6]. These models show that one can inadvertently include or exclude freezing drops from the analysis, which biases the results. The same models can be used to exclude or mitigate systematic biases, by refining the experimental design and the data selection.

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Observing the Liquid-Liquid Transition in Water Nanodroplets

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Simulation studies have identified water nanodroplets as potential systems in which to observe the second critical point of water and accompanying liquid-liquid phase transition that are believed to occur far below freezing and at high pressure. While their small size suppresses crystallization, it also provides a way to achieve high pressure through the curvature-induced Laplace pressure. Simulations using the TIP4P/2005 model demonstrated bulk-like behaviour, including density and compressibility anomalies, in nanodroplets containing only hundreds of molecules [1]. However, the high critical pressure of $P_c = 185$ MPa for TIP4P/2005 means that droplets achieving P_c (at a radius of approximately 2 nm and containing only a few hundred molecules) are too small to show a clear phase transition. By contrast, simulations with the WAIL model, for which $P_c \approx 50$ MPa, clearly show the transition between a low-density liquid (LDL) and a high-density liquid (HDL) for droplets containing N ~ 10,000 molecules [2]. We present new results based on an updated version of the model, rWAIL, that has an improved prediction of $P_c \approx 100$ MPa, and appears to show a LDL-HDL transition in droplets containing ~1000 molecules, implying that the transition should be observable in real water nanodroplets. Furthermore, we introduce He gas as a pressurizing medium to effect the LDL-HDL transition in larger rWAIL nanodroplets (see Fig. 1). We find that the solubility of He is significantly larger in LDL than in HDL, such that the concentration of He inside the nanodroplet, which normally increases with increasing pressure of the surrounding He gas, decreases during the nanodroplet's transition from LDL to HDL and thus may provide a convenient marker of the transition.

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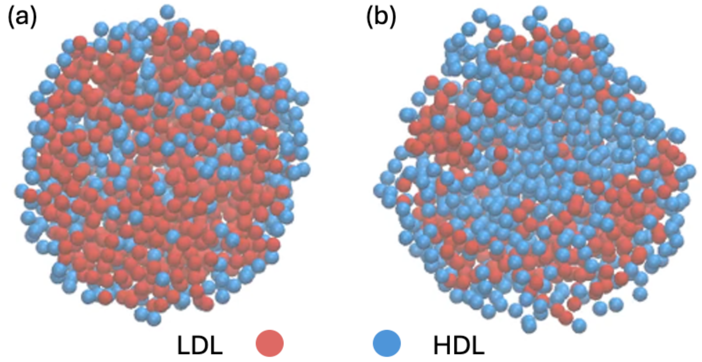

Fig. 1 Cross-sectional view of an N=2568 rWAIL nanodroplet at 200 K surrounded by He gas (not shown), with $P_{He} \approx 70$ MPa. Here, the droplet density strongly fluctuates between (a) LDL- and (b) HDL-dominant configurations.

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Observation of a dynamic transition in bulk supercooled water

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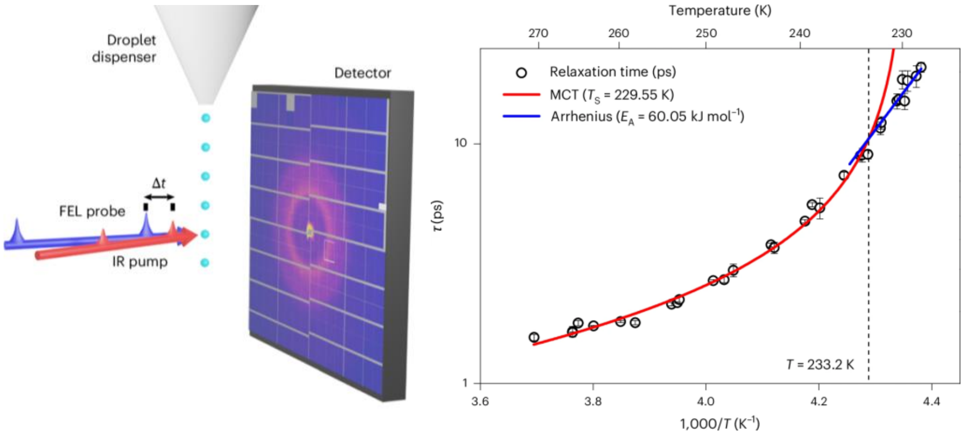
One of the longest standing mysteries of water is the rapid deceleration of its dynamic properties, such as viscosity and diffusivity upon cooling.(*1*) It has been conjectured, that water undergoes a dynamic crossover at some supercooled temperature, below which water's relaxation dynamics decelerate more gradually.(*2*) The nature of this transition has remained elusive, due to water rapidly freezing when cooled below the homogeneous nucleation temperature. We have utilized a novel methodology, making it possible to directly monitor relaxation dynamics in deeply supercooled water.(*3*) 15 μm sized droplets are cooled down to 228 K by evaporative cooling. Temperature jumps on the order of 1 K are induced by an IR-laser. The heating-induced structural relaxation is then probed by wide-angle x-ray scattering of FEL-pulses from SwissFEL. We clearly observe that the dynamics deviate from a power-law decrease below 233.2 K, indicating a dynamic transition. The relation of the transition to structural changes occuring in the solvent in this temperature range is discussed.



Left – scheme describing the pump probe experiment used to measure the timescale of structural relaxation in water. **Right –** Temperature dependence of the relaxation time, indicating a crossover from a power law to an Arrhenius regime.

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Liquid water is markedly different than liquid H_2X (X = S, Se, Te)

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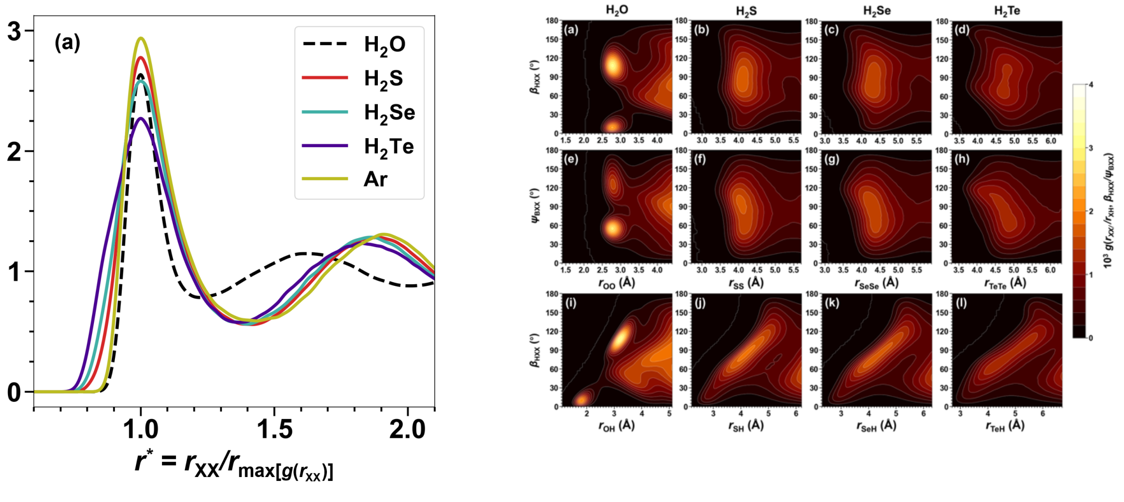
Among liquid water's many anomalous properties, the high melting, boiling and critical points compared to the ones of the rest of chalcogen hydrides (H_2S, H_2Se, H_2Te) are critical in ensuring the presence of water in the gas, liquid and solid forms on the surface of the earth to support aqueous-based life. Ab-initio molecular dynamics simulations for the liquid state of these systems using high-quality meta-GGA functionals, chosen to reproduce gold standard CCSD(T)/Complete Basis Set results for their small clusters, suggest marked differences in the properties of liquid water compared to H_2X (X = S, Se, Te). Angular distribution functions confirm the well-known result that each H_2O molecule averages 4-5 nearest-neighbors and an overall tetrahedral order, however they suggest that each H2X molecule averages ~12 nearest neighbors and significant departure from the tetrahedral structural motif. Furthermore, two-dimensional radial/angular distributions reveal subtle but consistent structural motifs, which progress from H_2S to H_2Te but are starkly different from those of water. Our results demonstrate that water forms an exceptionally different liquid from H_2S, H_2Se, and H_2Te, whereas the last three form exceptionally similar liquids to each other. The bonding scenarios in the liquid state of the heavier chalcogen hydrides is analyzed in terms of the competition between hydrogen and chalcogen bonds.



The radial distribution function *g*(XX), X = O, S, Se, Te, Ar in reduced coordinates at the halfway temperatures $T = T_m + (T_b - T_m)/2$, where T_m, T_B are the experimental melting and boiling temperatures for each system. (right). Coupled two-dimensional RDF/ADFs for the pairs (a-d) (r_{XX}, β_{HXX}), (e-h) (r_{XX}, ψ_{BXX}), and (i-l) (r_{XX}, β_{HXX}) in liquid H_2O (a, e, i), H_2S (b, f, j), H_2Se (c, g, k), and H_2Te (d, h, l) (right).

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Decoding hydrate formation: interfacial free energies and nucleation rates of methane and carbon dioxide from molecular simulation

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Clathrate hydrates are nonstoichiometric crystalline inclusion compounds in which small guest molecules—such as methane (CH_4) and carbon dioxide (CO_2)—are trapped within cages formed by a periodic, hydrogen-bonded host lattice [1,2]. These materials have attracted sustained fundamental and applied interest [1–4], motivated by their potential for CO_2 capture and by their relevance to energy resources, since natural hydrates are estimated to contain more CH_4 than conventional fossil-fuel reservoirs [5,6]. Here we show that simplified molecular models for water and guest species can still yield valuable insight into a key quantity governing hydrate nucleation and crystal growth: the hydrate–water interfacial free energy [7]. This interfacial free energy is central to hydrate formation in settings ranging from energy storage to CO_2 sequestration and climate-related processes, yet it remains poorly constrained experimentally due to large uncertainties. Reported interfacial free energies for CH_4 and CO2 hydrates range from 28–40 and 22-34 mJ/m^2, respectively [8–10], values that are comparable to that of the ice Ih–water interface (~32 mJ/m^2) [11]. We present direct molecular simulations of the CO_2 and CH_4 hydrate–water interfacial free energies using two independent extensions of the mold-integration method, which generate planar interfaces and evaluate the reversible work of formation [12,13]. Our results indicate that CH_4 hydrate has a markedly higher interfacial free energy than CO_2 hydrate, consistent with their contrasting nucleation kinetics [12-16]. The predicted CH_4 value (~40 mJ/m^2) matches the upper end of experimental estimates, whereas CO_2 hydrate and ice Ih remain close to ~30 mJ/m^2. These direct, theory-independent benchmarks sharpen our understanding of hydrate formation mechanisms and provide reliable targets for predictive modeling and hydrate-based technologies.

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Microscale Investigation of CO_2 Hydrate Formation in Saline Solutions by Optical Microscopy and Raman Spectroscopy: Implications for Hydrate-Based Desalination

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Hydrate-based desalination has emerged as a promising approach for freshwater production, relying on the formation of gas hydrates that selectively incorporate guest molecules while excluding dissolved salts from the crystalline lattice. However, the microscale processes governing hydrate nucleation, growth, and salt redistribution in saline environments remain poorly understood.

Here we investigate CO_2 hydrate formation in NaCl solutions using optical microscopy coupled with micro-Raman spectroscopy in high-pressure transparent micro-capillary reactors. This combined optical and spectroscopic approach enables direct in situ observation of hydrate nucleation and growth at the micrometre scale, while simultaneously providing molecular-level information on both guest (CO_2) and host (water) environments.

Our results show that the initial CO_2 dissolution state controls hydrate nucleation pathways and spatial growth patterns, resulting in distinct formation regimes between partially and fully CO_2-saturated solutions.[1] Increasing salinity further promotes heterogeneous hydrate–brine coexistence and influences salt redistribution during hydrate formation, while altering the hydrogen-bond network of the surrounding aqueous phase.[2]

Raman signatures from the CO_2 Fermi dyad and O–H stretching region reveal spectroscopic markers of hydrate-rich domains, salt exclusion, and progressive brine enrichment during crystallization. These observations provide new insight into the microscale mechanisms governing hydrate formation in saline systems and their implications for hydrate-based desalination processes.

Keywords: Hydrate-based desalination, salt exclusion, micro-Raman spectroscopy, CO_2 hydrates, micro-capillary reactors

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Effect of Gas Type and Additives Based on Natural Raw Materials on Nucleation, Growth, and Agglomeration of Gas Hydrates

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Changes in temperature and pressure during the production, collection, processing and transportation of oil and gas can lead to the condensation of water, the formation of ice and/or gas hydrates. When developing agents to control hydrate formation in the modern context, it is important to ensure that they are effective and environmentally friendly. Understanding how the composition and structure of these agents influence the kinetic parameters of hydrate nucleation and growth enables the development of environmentally safe agents based on natural raw materials.

This study presents a systematic investigation of the nucleation, growth and agglomeration of methane (CH_4; sI), carbon dioxide (CO_2; sI) and methane/propane (CH_4/C_3H_8; sII) hydrates in a batch autoclave [1] and rocking cells. The study found that the nucleation and growth rates of sII hydrates (CH_4/C_3H_8) are lower than those of sI hydrates (CH_4, CO_2), with CO_2 hydrate exhibiting the highest formation rate. The influence of reagents based on cellulose, agarose, and clays was also investigated. Promising forms of nanofibrillar cellulose that exhibit the properties of kinetic inhibitor, as well as modified agarose microspheres that act as hydrate formation promoter, were identified. Developing environmentally friendly reagents for controlling hydrate formation based on natural materials will help to achieve resource-efficient energy goals and reduce the carbon footprint of the oil and gas industry.

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Nuclear Quantum Effects on the Equation of State of Water: Insights from the Potential Energy Landscape Formalism

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We apply the potential energy landscape (PEL) formalism for quantum liquids together with path-integral computer simulations to derive the equation of state (EOS) of equilibrium and supercooled (q-TIP4P/F) water across a broad temperature–pressure range. Our PEL-EOS, which explicitly includes nuclear-quantum effects (NQE), reproduces path-integral simulations results closely, especially near water's liquid–liquid critical point (LLCP). A comparison with classical water shows that NQE shift the phase diagram to lower temperatures and slightly lower pressures: $\Delta T_c \approx -18$ K, $\Delta P_c \approx -49$ MPa, and a minor change in the critical density ($\Delta \rho_c \approx -0.002$ g·cm−3). These shifts approximate the maximum LLCP displacement expected from $H_2O \rightarrow D_2O \rightarrow T_2O$ isotope substitution. NQE also modify the density and liquid–liquid spinodal loci in the P–T plane. We find the PEL of (q-TIP4P/F) water to be Gaussian, enabling direct evaluation of the configurational entropy $S_{IS}(T,V)$ and the Kauzmann temperature $T_K(V)$; NQE reduce T_K by ~5–20 K depending on density. This reduction correlates with an increase in the diffusion coefficient D at low T when quantum fluctuations are included. Notably, the Adam–Gibbs relation between D and SIS holds across all densities studied. From the perspective of the PEL formalism, NQE alter the curvature of PEL basins while leaving inherent structures (IS) effectively unchanged (isomorphic to the classical IS). The PEL-based approach presented is versatile and physically transparent, and can be applied to compute free energies and EOS for other quantum liquids.

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Thermodynamics of Liquid Water via Time-Series Analysis

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By analysing the temporal evolution of the hydrogen-bond network (HBN) topology in simulations of liquid water across a range of thermodynamic conditions, we show that the dynamics of microscopic topological motifs within the HBN encode the system's macroscopic thermodynamic behaviour. Moreover, we demonstrate that time-series analysis of these dynamics enables the prediction of thermodynamic properties in regions of the phase space that were not directly sampled in our simulations.

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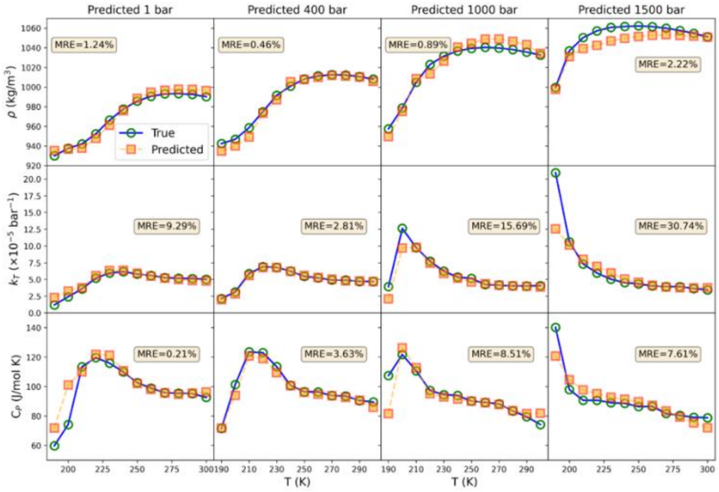

Figure 1 Predicted (squares) vs simulated (circles) thermodynamic response functions.

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Dynamical properties of high-pressure water by Machine Learning based Molecular Dynamics

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We present a study of liquid water in the pressure range up to 4GPa and temperature up to 480K by Molecular Dynamics simulation employing a machine learned many-body force field with the MACE protocol [1]. We have trained the MACE force field on density functional theory (DFT) energies, forces and stress obtained by the revPBE-D3 approximation [2] on nuclear configurations in the relevant density range.

Our predicted structural and dynamical properties of compressed water are in good agreement with experimental measurements [3,4]. The nature of the hydrogen bond network and its persistence with pressure is investigated.

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Solvation mechanisms and transport properties in supercritical water from ab Initio machine-learning molecular dynamics

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Using ab initio–trained machine-learning molecular dynamics simulations, we show that water behaves as a porous, flexible fluid under supercritical conditions. Entering the supercritical regions, large volumes depleted of H_2O emerge.

These strong density fluctuations, along with the breaking of hydrogen bonding [1,2], make the supercritical water (SCW) network highly flexible. Consequently, SCW solvates solutes at higher concentrations than water under ambient conditions. For example, conductivity measurements in volcanic systems (600-800 K, 1-1.5 kbar) suggest the presence of charged fluids [3], in which SCW can dissolve up to ~50 wt% NaCl [4], far exceeding the ~3.5 wt% typical of seawater.

To elucidate solvation mechanisms in SCW and highlight the differences from ambient conditions [5], we compare the probability of forming H_2O-depleted regions in pure SCW and in SCW with varying concentrations of hydrophobic (10–20 wt% CO_2) and hydrophilic (10–20–40 wt% NaCl) species. We find that the interplay between NaCl clusters and H_2O-depleted regions regulates charge transport. Our results offer a new perspective on solvation in SCW. In addition, we provide insights into the conductivity of Na-Cl–H_2O fluids in volcanic plumbing systems to improve geophysical models of supercritical reservoirs.

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Solvent Mediated Regulation of FUS Biomolecular Condensates

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The compartmentalization of intrinsically disordered proteins through liquid-liquid phase separation into membrane-less biomolecular condensates regulates cellular biochemical processes. Environmental conditions such as pH, temperature, and salt concentration have been shown to impact condensate formation, sometimes resulting in dissolution of these protein enriched, liquid-like droplets. Yet, the molecular organization within condensates remains largely unknown and how their molecular properties change with environmental conditions has not been explored. Here, the role of solvation dynamics in the liquid-liquid phase separation of the intrinsically disordered protein fused in sarcoma (FUS) is probed. Characterization of the hydrogen bonding network with Terahertz spectroscopy reveals that water solvating hydrophobic groups is stripped away in the FUS biomolecular condensates. Additionally, water left inside of the condensates is highly constrained, indicative of a population of bound hydration water. Solvent conditions and FUS protein sequency alter hydration dynamics in condensations. The strength of the hydrogen bonding network of bound hydration water is cation specific, while protein modifications impact both the population and strength of hydration water. Together, these results reveal that protein-water interactions regulate the stability of FUS condensates, ultimately shedding light on the molecular properties that govern the organization of condensates.

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Remnants of criticality in hydrophobicity

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Hydrophobic interactions play a crucial role in various biological and chemical processes, yet their underlying mechanics are not fully understood. We take a perspective that links macroscopic drying with the microscopic solute-solute interactions, computing potentials of mean force between solutes of various radii using metadynamics. Our results show that the resulting effective interactions are stronger at higher temperatures, a trend controlled by the expansion of the solvation shell and connected to the physics of critical drying. We will discuss a minimal morphometric model that rationalises this behaviour in terms of local inhomogeneities of the density field and strength of the water solute interactions. The proposed model, therefore, links near-critical behaviour or pre-transition physics and local density inhomogeneities to the emergence of hydrophobic forces, characterising their strength and range within a generic, solvent-independent framework. This contrasts with the conventional interpretation of the hydrophobic effect, which emphasises the role of water-specific hydrogen-bond networks.

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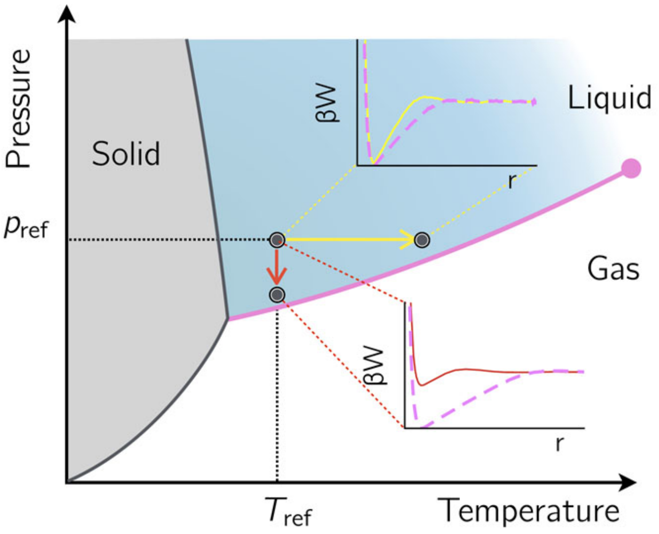

Schematic phase diagram of water shows thermodynamic routes to evaluate solute-solute interactions. As we approach coexistence, surface criticality affects the potential of mean force W(r), thereby strengthening the hydrophobic attraction.

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On the entropic driving force of the contact-minimum configuration of two large Lennard-Jones particles in TIP4P/2005 water

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In a recent work by Naito, Sumi, and Koga, NSK, the analysis of long molecular dynamics trajectories showed that the formation of the contact-minimum, *cm*, configuration of two Lennard-Jones particles in the TIP4P/2005 water model [2] is driven by entropy, regardless of the particle diameter [1]. This result is striking as it is in contrast to the claim that the driving force should be enthalpic for large spherical particles. The observed entropy gain must arise from water, and its molecular origin needs to be clarified. In the past, one of us devised a simple theoretical approach based on the geometric features of the *cm* configuration [3]. The latter has a smaller solvent-excluded volume than the two particles when they are separated by a large distance. The decrease in solvent-excluded volume, which can be measured by the decrease in water accessible surface area, produces an increase in the volume available to water molecules, which translates into an increase in their translational entropy. This entropy gain drives the formation of the *cm* configuration. Applying this geometric approach to the largest LJ particles investigated by NSK yields values for the water-mediated thermodynamic functions consistent with those obtained through molecular dynamics simulations [4].

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Coordination-resolved H–O Bond Properties and Thermal Anomalies

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Based on the hydrogen-bond cooperative polarization (HBCP) theory [1] and perturbation-resolved electron-phonon spectroscopy (PRS)[2], we treat O:H–O as a cooperatively responsive unit coupled by O↔O repulsion (Fig. 1a). Our experiments reveal:

1. **Coordination-induced bond stiffening**: Molecular undercoordination shortens and stiffens H–O bonds via O↔O repulsion, from bulk water (1.00 Å, 3.97 eV, 3200 cm^{-1}) to the isolation limit (0.90 Å, 5.10 eV, 3608 cm^{-1}) (Table 1).
2. **Sign-reversible thermal response:** The coefficient α(z,T) drops from $+500.0\times10^{-3}$ (bulk) to -8.4×10^{-3} (isolated molecules), marking the transition from anomalous "heating-induced contraction" to classical "heating-induced expansion." Weakly coupled dangling bonds (>298 K) and interfacial water (>340 K) exhibit red shifts (thermal expansion), opposite to bulk behavior (Fig. 1b–d).
3. **Anti-correlated bond relaxation**: O:H and H–O respond oppositely to perturbations, with O:H relaxing more extensively.

These findings establish O↔O repulsion as the governing mechanism and H–O frequency as a quantitative probe, advancing understanding of water anomalies through coordination imperfection and many-body cooperativity, with broad implications for hydrogen-bonded systems.

Table 1 PRS measurements (vibration frequency ω_H and thermal response coefficient α) and HBCP theoretical calculations (bond length d_H and energy E_H, O–O distance d_O and repulsive coupling strength E_O).

		PRS Measurements			HBCP Parametrization			
H-O	**CN/ Coupling**	ω_H (cm^{-1})	α(T) $\times10^{-3}$	α(P)	d_H (Å)	d_O (Å)	$-E_H$ (eV)	E_O (eV)
H_2O/CL-20	**~0**	3608	-8.4		0.9007	2.9383	5.10	0.05
Dangling		3610						
Interface	**weak**	3450			0.9327	2.8620	4.70	0.40
Bulk	**full**	3200	+500.0		1.0004	2.6950	3.97	1.13

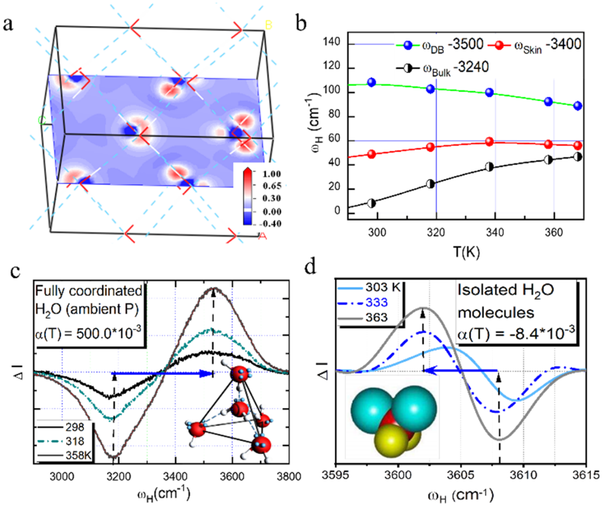

Fig. 1 H–O vibrational frequencies and thermal responses. (a) Charge density distribution revealing the O:H–O unit and O↔O repulsion. (b) The $\omega_H(z,T)$ resolves the bulk (~3240 cm^{-1}), interface (~3440 cm^{-1}), and dangling bonds (~3610 cm^{-1}). Positive slopes indicate heating-induced contraction. Weakly coupled dangling bonds (>300 K) and interfacial water (>340 K) exhibit classical thermal expansion. (c) Bulk water: blue shift (contraction). (d) Near-isolated H_2O@CL-20: red shift and sign reversal (expansion). The response coefficient $\alpha(T) = d\ln\omega/d\ln T = T_i(\omega_f-\omega_i)/[\omega_i(T_f-T_i)]$. For (d): $T_i = 303$ K, $T_f = 363$ K, $\omega_i = 3608\ cm^{-1}$, $\omega_f = 3603\ cm^{-1}$ (PRS resolution: 3 cm^{-1}).

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Some comment on ldl and hdl state of liquid water

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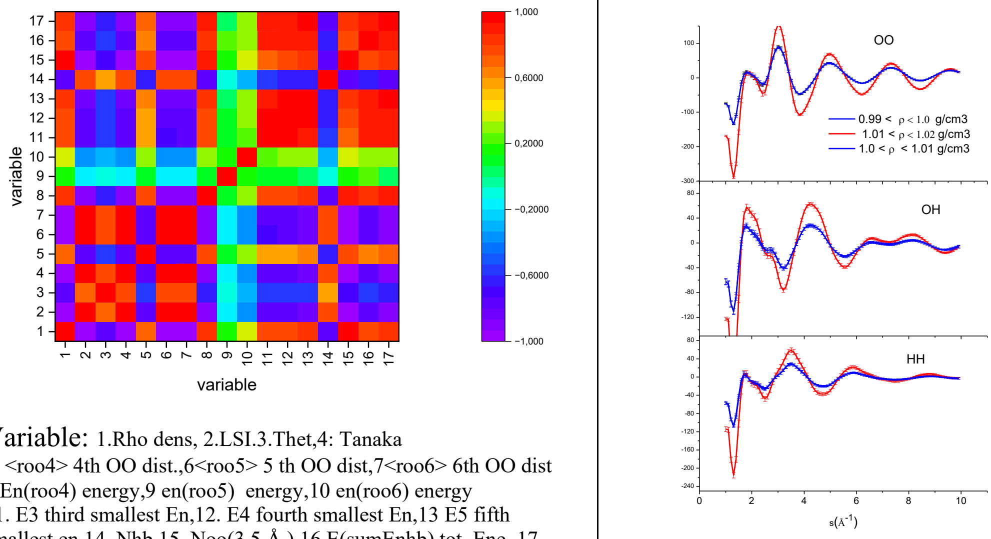
Liquid water has unique and anomalous properties due to its ability to form a hydrogen-bonded space-filling network. The liquid state can be characterised by a complex structure that oscillates between two classes of local environments, namely low density fluid (high energy, low entropy) and high density fluid (low energy, high entropy). The most accepted hypothesis to explain the anomalous properties of water under deeply supercooled conditions is that there exists a second critical point. According to molecular dynamics simulations, this transition is first order and occurs rapidly at increased pressure In this study, a long molecular dynamics simulation was analysed using various local (local structural index, tetrahedrality, Tanaka parameter, hydrogen bonded neighbour number, and network descriptors (communicability..).

We show that the correlation between the mean of these descriptors on a configuration is high (> 0.8, right fig.), and the application of a clustering procedure clearly yields high and low density states. Contrary to this observation, when the actual value of these descriptors is applied on separated parts of the systems, the clustering procedure does not show a well-defined decomposition. We think, that coexistence of ldl and hdl regions is hindered at small systems, e.g., 300 molecules. Our calculations partly based on the OO structure function clearly show a sudden phase transition between 1.01 and 1.02 g/cm^3, left figure a.



Variable: 1.Rho dens, 2.LSI.3.Thet,4: Tanaka
5. <roo4> 4th OO dist.,6<roo5> 5 th OO dist,7<roo6> 6th OO dist
8 En(roo4) energy,9 en(roo5) energy,10 en(roo6) energy
11. E3 third smallest En,12. E4 fourth smallest En,13 E5 fifth smallest en,14. Nhb,15. Noo(3.5 Å),16 E(sumEnhb) tot. Ene.,17. E(sumE(roo<3.5 Å))

Figure caption: a: Pearson correlation coefficient among the characteristics variable; b: Partial structure function of liquid water in two different phase
[1]

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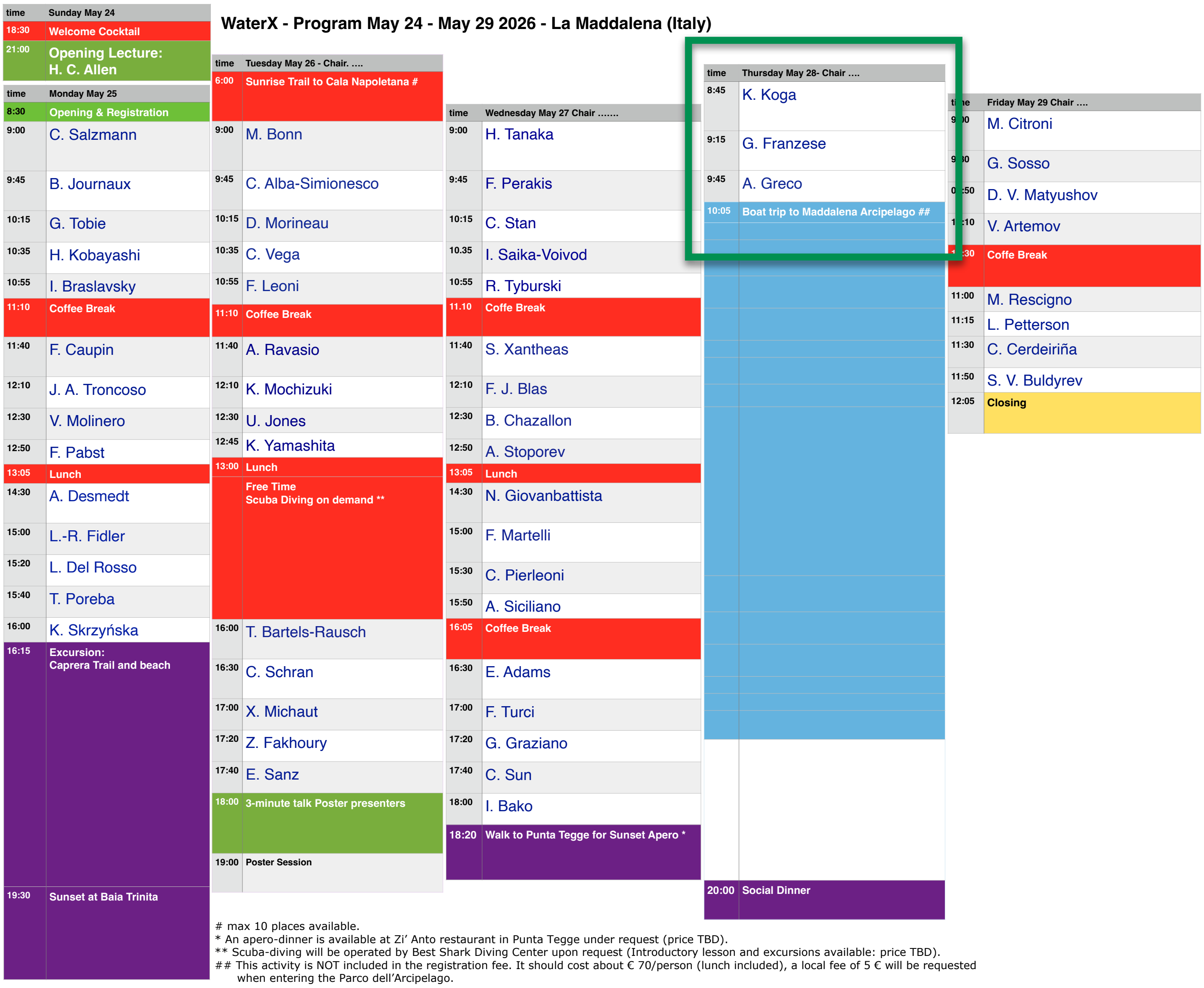

WaterX - Program May 24 - May 29 2026 - La Maddalena (Italy)

time	Sunday May 24
18:30	Welcome Cocktail
21:00	**Opening Lecture: H. C. Allen**

time	Monday May 25
8:30	Opening & Registration
9:00	C. Salzmann
9:45	B. Journaux
10:15	G. Tobie
10:35	H. Kobayashi
10:55	I. Braslavsky
11:10	Coffee Break
11:40	F. Caupin
12:10	J. A. Troncoso
12:30	V. Molinero
12:50	F. Pabst
13:05	Lunch
14:30	A. Desmedt
15:00	L.-R. Fidler
15:20	L. Del Rosso
15:40	T. Poreba
16:00	K. Skrzyńska
16:15	Excursion: Caprera Trail and beach
19:30	Sunset at Baia Trinita

time	Tuesday May 26 - Chair. ....
6:00	Sunrise Trail to Cala Napoletana #
9:00	M. Bonn
9:45	C. Alba-Simionesco
10:15	D. Morineau
10:35	C. Vega
10:55	F. Leoni
11:10	Coffee Break
11:40	A. Ravasio
12:10	K. Mochizuki
12:30	U. Jones
12:45	K. Yamashita
13:00	Lunch
	Free Time Scuba Diving on demand **
16:00	T. Bartels-Rausch
16:30	C. Schran
17:00	X. Michaut
17:20	Z. Fakhoury
17:40	E. Sanz
18:00	3-minute talk Poster presenters
19:00	Poster Session

time	Wednesday May 27 Chair ....
9:00	H. Tanaka
9:45	F. Perakis
10:15	C. Stan
10.35	I. Saika-Voivod
10:55	R. Tyburski
11.10	Coffee Break
11:40	S. Xantheas
12:10	F. J. Blas
12:30	B. Chazallon
12:50	A. Stoporev
13:05	Lunch
14:30	N. Giovanbattista
15:00	F. Martelli
15:30	C. Pierleoni
15:50	A. Siciliano
16:05	Coffee Break
16:30	E. Adams
17:00	F. Turci
17:20	G. Graziano
17:40	C. Sun
18:00	I. Bako
18:20	Walk to Punta Tegge for Sunset Apero *

time	Thursday May 28- Chair ....
8:45	K. Koga
9:15	G. Franzese
9:45	A. Greco
10:05	Boat trip to Maddalena Arcipelago ##
20:00	Social Dinner

ti e	Friday May 29 Chair ....
9 00	M. Citroni
9 30	G. Sosso
0 :50	D. V. Matyushov
1 :10	V. Artemov
:30	Coffe Break
11:00	M. Rescigno
11:15	L. Petterson
11:30	C. Cerdeiriña
11:50	S. V. Buldyrev
12:05	Closing

\# max 10 places available.
* An apero-dinner is available at Zi' Anto restaurant in Punta Tegge under request (price TBD).
** Scuba-diving will be operated by Best Shark Diving Center upon request (Introductory lesson and excursions available: price TBD).
\#\# This activity is NOT included in the registration fee. It should cost about € 70/person (lunch included), a local fee of 5 € will be requested when entering the Parco dell'Arcipelago.

Some Topics on Water-Mediated Interaction

Kenichiro Koga
Okayama University, Japan

Water-mediated interactions, including hydrophobic interactions, are more difficult to measure quantitatively than the solubility of solutes in water. Nevertheless, to predict or control various processes occurring in aqueous solutions—such as the self-assembly of amphiphilic molecules and the coil-globule transition in water-soluble polymers—it is critical to understand quantitatively how these interactions vary with changes in temperature, the addition of cosolvents or ions, or the chemical properties of the solute molecules.

In this talk, we discuss three topics regarding water-mediated interactions based on results from molecular simulations and theoretical modeling. First, we examine the interplay between the coil-globule transition of a single polymer in water and the aggregation of such polymers. Specifically, we investigate how conformational changes in a polymer chain affect the cloud point of the system [1]. Second, we examine how water-mediated interactions between hydrophobic particles in electrolyte solutions change as the nature of the ions shifts from strongly salting the solute out to strongly salting it in. The salting-out ability is measured by the Setschenow coefficient, K_s, while the ability to increase the effective attraction between solute particles is measured by the salt-enhanced association (SEA) coefficient, C_I [2]. Simulation results reveal an interesting nonlinear behavior in C_I as a function of K_s, as shown in Fig. 1 and as anticipated by theoretical calculations [2]. Third, we discuss water-mediated interactions between ions and interfaces.

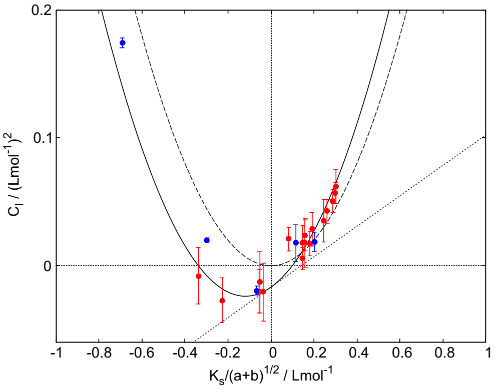

Fig. 1. The salt-enhanced association (SEA) coefficient C_I versus the Setschenow coefficient K_s for aqueous solutions of methane with various ions and cosolvents.

[1] J. Komatsu, K. Koga, and J. Berx, J. Chem. Phys. **163**, 191101 (2025).

[2] R. Okamoto and K. Koga, J. Phys. Chem. B, **86**, 12820 (2021).

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Water and ionic aqueous solutions under extreme conditions through a REST Model

Giancarlo Franzese
Departament de Física de la Matéria Condensada, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain
Institut de Nanociencia i Nanotecnologia (IN2UB), Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain

We introduce a REST (Reliable, Efficient, Scalable, Transferable) molecular model of water built from quantum-derived many-body parameters, validated against advanced polarizable models and experimental data. The model quantitatively reproduces water thermodynamics under extreme conditions, matching the equation of state and response functions up to 50 MPa and across a 100 K range around ambient temperature [1, 2].

Its transferability extends to aqueous ionic solutions, enabling microscopic insight into how ions reshape the hydrogen bond network [3]. This includes a quantitative assessment of the Jones–Dole viscosity relation, connected to experimental trends [4].

The model's computational efficiency allows large-scale simulations approaching micrometer-sized droplets with modest resources [5]. Its combination of accuracy and scalability provides a powerful tool for exploring water anomalies and for applications in bionano systems and complex fluid environments.

[1] L. E. Coronas, and G. Franzese, "Phase behavior of metastable water from large-scale simulations of a quantitatively accurate model near ambient conditions: The liquid-liquid critical point", Journal of Chemical Physics 2024, 161, 164502.

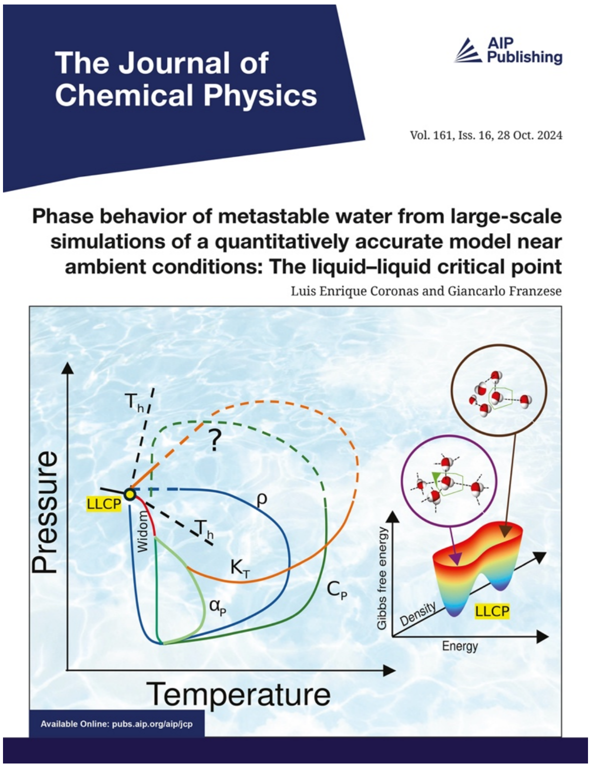
[2] L. E. Coronas, O. Vilanova, and G. Franzese, "A transferable molecular model for accurate thermodynamic studies of water in large-scale systems", Journal of Molecular Liquids 2025, 434, 128032.

[3] S. Pelosso, S. Panzuela, F. de los Santos, and G. Franzese, *in preparation*, 2026.

[4] T. Corridoni, R. Mancinelli, M. A. Ricci, and F. Bruni, "Viscosity of Aqueous Solutions and Local Microscopic Structure", The Journal of Physical Chemistry B 2011, 115, 14008–14013.

[5] L. E. Coronas, O. Vilanova, and G. Franzese, "Efficient parallel algorithms for Monte Carlo simulations of millions of water molecules in the fluid phase", Frontiers in Nanotechnology 2025, 7, 1637828.

`gfranzese@ub.edu`



The Journal of
Chemical Physics

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Vol. 161, Iss. 16, 28 Oct. 2024

Phase behavior of metastable water from large-scale simulations of a quantitatively accurate model near ambient conditions: The liquid–liquid critical point

Luis Enrique Coronas and Giancarlo Franzese

Available Online: pubs.aip.org/aip/jcp

Cover of Ref. [1]

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Ultrafast Water Dynamics at Aqueous Electrolyte Interfaces

Alessandro Greco
Max Planck Institute for Polymer Research

The electric double layer (EDL) formed at electrolyte interfaces plays a central role in electrochemistry, energy storage, and interfacial chemistry. However, the molecular-scale dynamics governing EDL relaxation remain poorly understood, particularly at high electrolyte concentrations where ion–ion correlations and ion–solvent interactions may lead to deviations from classical mean-field descriptions.

Here we present an all-optical approach to probe ultrafast EDL dynamics at aqueous interfaces. Using time-resolved vibrational sum-frequency generation (TR-vSFG) spectroscopy, we drive the system out of equilibrium via an infrared-induced temperature jump (T-jump) and monitor the interfacial response with sub-picosecond temporal resolution. The orientation of interfacial water molecules serves as a reporter of the transient electric field associated with the EDL.

Experiments at the air–electrolyte interface reveal relaxation dynamics on timescales of tens to hundreds of picoseconds, reflecting ion desorption and rearrangement. Non-equilibrium molecular dynamics simulations and analytical modeling show that the dynamics are primarily governed by ionic conduction and remain consistent with mean-field predictions (Debye–Falkenhagen theory), even at high concentrations.

[1] A. Greco et al., Science 2025, 388, 405 – 410.

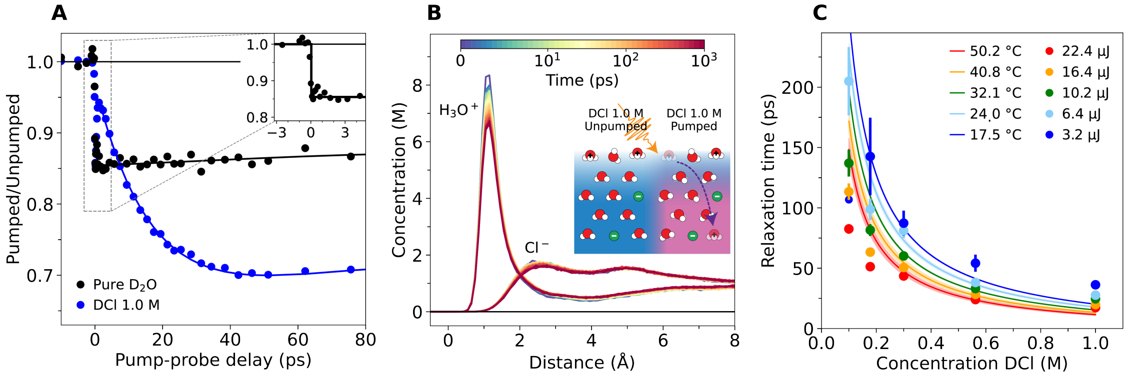

Fig. 1. (A) Time-resolved traces of integrated vSFG spectra following excitation by an IR pump pulse with an energy of ~20.0 μJ. (B) Time evolution of ion distributions from MD simulations after the T-jump. (C) Experimental time constants for EDL dynamics (solid circles) at different excitation fluences and DCl concentrations, compared with classical Debye–Falkenhagen relaxation times calculated at the corresponding final temperatures (lines).

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WaterX - Program May 24 - May 29 2026 - La Maddalena (Italy)

time	Sunday May 24
18:30	**Welcome Cocktail**
21:00	**Opening Lecture: H. C. Allen**

time	Monday May 25
8:30	**Opening & Registration**
9:00	C. Salzmann
9:45	B. Journaux
10:15	G. Tobie
10:35	H. Kobayashi
10:55	I. Braslavsky
11:10	**Coffee Break**
11:40	F. Caupin
12:10	J. A. Troncoso
12:30	V. Molinero
12:50	F. Pabst
13:05	**Lunch**
14:30	A. Desmedt
15:00	L.-R. Fidler
15:20	L. Del Rosso
15:40	T. Poreba
16:00	K. Skrzyńska
16:15	**Excursion: Caprera Trail and beach**
19:30	**Sunset at Baia Trinita**

time	Tuesday May 26 - Chair. ....
6:00	**Sunrise Trail to Cala Napoletana #**
9:00	M. Bonn
9:45	C. Alba-Simionesco
10:15	D. Morineau
10:35	C. Vega
10:55	F. Leoni
11:10	**Coffee Break**
11:40	A. Ravasio
12:10	K. Mochizuki
12:30	U. Jones
12:45	K. Yamashita
13:00	**Lunch**
	Free Time Scuba Diving on demand **
16:00	T. Bartels-Rausch
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18:20	**Walk to Punta Tegge for Sunset Apero ***

time	Thursday May 28- Chair ....
8:45	K. Koga
9:15	G. Franzese
9:45	A. Greco
10:05	**Boat trip to Maddalena Arcipelago ##**
20:00	**Social Dinner**

time	Friday May 29 Chair ....
9:00	M. Citroni
9:30	G. Sosso
09:50	D. V. Matyushov
10:10	V. Artemov
10:30	**Coffe Break**
11:00	M. Rescigno
11:15	L. Petterson
11:30	C. Cerdeiriña
11:50	S. V. Buldyrev
12:05	**Closing**

\# max 10 places available.
* An apero-dinner is available at Zi' Anto restaurant in Punta Tegge under request (price TBD).
** Scuba-diving will be operated by Best Shark Diving Center upon request (Introductory lesson and excursions available: price TBD).
\#\# This activity is NOT included in the registration fee. It should cost about € 70/person (lunch included), a local fee of 5 € will be requested when entering the Parco dell'Arcipelago.

Water Under Extreme Conditions from Discovery to Publication

Margherita Citroni, phD
Chief Editor for Materials Science and Physical Chemistry, *Nature Communications*
Nature Portfolio
Heidelberger Platz 3, 14197 Berlin, Germany

Water has long fascinated scientists as a structurally simple molecule exhibiting an unusually rich range of behaviors. These include anomalous thermodynamic properties linked to experimentally inaccessible regions of the phase diagram, multiple stable and metastable phases with varying degrees of structural order, and dynamics that are strongly influenced by solutes or confinement. Beyond its fundamental interest, water is a major constituent of terrestrial and extraterrestrial environments, where its physical properties play a central role in shaping physical, chemical, and biological processes. It is therefore unsurprising that studies of water under extreme conditions continue to feature prominently in influential journals.

In a field with such multidisciplinary reach, communicating research findings to editors, referees, and readers can be challenging. More broadly, scientific progress is driven by advances of all scales that are robust, clearly reported, and open to further development, and the impact of research depends at least as much on these qualities as on the extraordinariness of the findings.

In this talk, we will explore what editors in the Nature portfolio look for when evaluating the impact of a manuscript, with particular focus on the topics of this meeting. We will also discuss best practices in data presentation with the aim of maximizing the clarity, durability, and reach of published research. Questions and discussion will be encouraged throughout the talk.

margherita.citroni@nature.com, https://www.nature.com/ncomms/

First Steps Toward Understanding Ice Formation in Plants

Gabriele C. Sosso
The University of Warwick

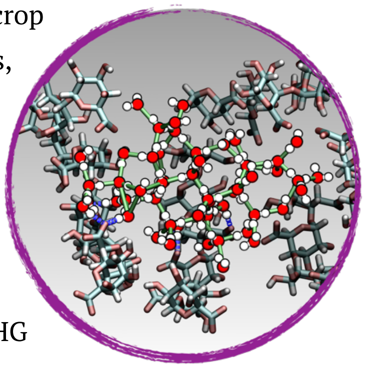

***Figure 1** - Ice nucleus forming at the interface with the pectin network*

Understanding how ice forms in plants is crucial to reducing crop losses amid increasing climate extremes. Unlike in animal tissues, the microscopic details of ice formation within plant cell walls remain poorly understood [1,2]. Here, we combine plant biology experiments and molecular simulations to investigate the crosslinking of homogalacturonan (HG) pectin under different functionalization states (deprotonated, protonated, methyl esterified). We show that the degree and nature of HG crosslinking strongly affect cell wall porosity, as revealed by experiments supported by mathematical modelling [3]. This porosity, in turn, governs the rate of ice propagation through plant tissue. Both cold acclimation and Ca^{2+} supplementation - which enhance HG crosslinking - improve frost resistance similarly. Simulations further indicate that while HG alone is a weak ice nucleator, ordered HG networks may promote ice formation (see Fig.1). Conversely, excess hydration reverses the inhibitory effect of crosslinking due to swelling. Molecular dynamics results reveal that HG crosslinking controls pore size and restricts ice growth via the Gibbs–Thomson effect, providing a physical basis for freezing tolerance through cell wall remodeling [4]. These findings highlight how water regulates the topology of pectin in the cell walls and how plants regulate ice formation by tuning pectin architecture, thus suggesting new strategies for improving frost resistance in crops.

[1] Physiological and Molecular Mechanisms of Freezing in Plants, Phyton-Int. J. Exp. Bot. **94**, 1601 (2025).

[2] H. Shikata, A. Yoshinari, M. Asaoka, and D. Takahashi, Memory in the wall: expanding our understanding of the roles of plant cell walls, New Phytol. **249**, 56 (2026).

[3] I. Obomighie et al., Understanding pectin cross-linking in plant cell walls, Commun. Biol. **8**, 72 (2025).

[4] I. Obomighie, I. J. Prentice, C. L. Box, F. Bachtiger, N. Ramsay, T. F. Whale, G. Tribello, T. J. Hawkins, G. C. Sosso, and H. Knight, Cold Acclimation Enhances Plant Cell Wall Pectin Crosslinking to Limit Ice Propagation, (unpublished).

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Mobility of water and ions in water

Dmitry V. Matyushov
Arizona State University, Department of Physics

Translational and rotational molecular diffusion are driven by fluctuating molecular forces, with the main components originating from van der Waals (vdW) and electrostatic forces. They turn out to be remarkably strongly correlated, both statistically and dynamically. Exact compensation relations between electrostatic and vdW forces are found to enhance diffusivity of water molecules in the bulk and of dissolved electrolyte ions [1,2]. The compensation relation fails for asymmetric ions, when the centers of vdW and electrostatic forces are geometrically separated. An asymmetric ion becomes an active Brownian particle, with an uncompensated force in its body frame. The friction is dramatically increased by electrostatic torques and diffusivity substantially (by a factor of 300 in our simulations) drops compared to spherical ions [3]. We also study non-Gaussian translational dynamics of water by MD simulations. Translational non-Gaussian parameter and rotational/translational relaxation times follow master curves produced by either changing temperature or liquid's dipole moment [2]. We thus find that electrostatics determine many non-standard dynamical features of low-temperature polar liquids. We find that collective dielectric response of polar liquids can be calculated directly from the single-particle dynamics. This perspective is allowed be near equality of single-particle and collective memory functions of rotational dynamics. Our recent MD simulations report rotational memory functions for the first time [4].

[1] T. Huang et al, Phys. Rev. Lett. 135 (2025) 028002.

[2] M. M. Pirnia and D. V. Matyushov, ChemRxiv (2026) 2026-t369k.

[3] S. M. Sarhangi and D. V. Matyushov, unpublished.

[4] D. Asthagiri and D. V. Matyushov, arXiv 2601.1022 (2026).

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Electrodynamics of Water in 1-nm Channels

Dr. Vasily Artemov
Hamburg University of Technology (TUHH), 21073 Hamburg, Germany

Water behavior at the nanoscale triggers cutting-edge technologies in energy, sensing, cooling, filtration, fluidics, and bioengineering. In this talk, I'll focus on the electrodynamics of confined water. I'll discuss, on equal footing, the experimental dielectric properties of water and ice from bulk to single-digit nanoconfinement and across direct current to terahertz [1]. I'll highlight previously overlooked mechanisms, including proton-mediated relaxation [2] and confinement-enhanced proton conductivity [3]. These findings open the door for topological effects, rather than chemical composition, to enhance the performance of electrochemical energy systems [4]. Specifically, I'll present a prototype supercapacitor made entirely from abundant clay materials with water as the sole electrolyte [5]. The robustness and scalability of this technology pave the way for broader applications, such as nanofluidics, fuel cells, and cooling systems. While the primary focus of the talk is on the electrodynamics of confined water, the fundamental insights will interest a wide audience of water researchers.

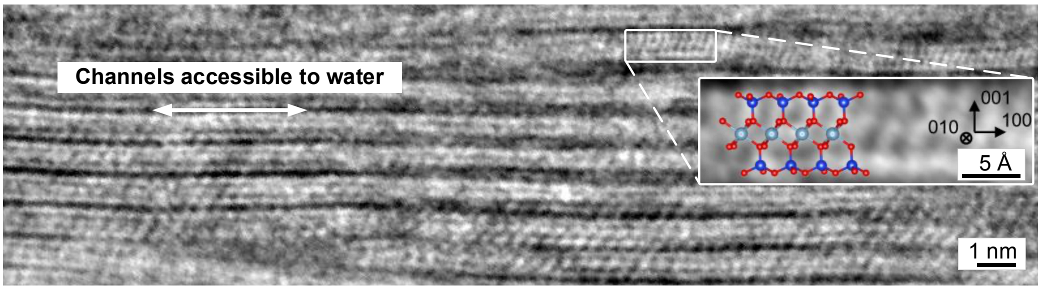

Figure 1: Transmission electron microscopy (TEM) image of clay heterostructure cross section with parallel orientation of individual flat crystalline flakes forming 2D-like channels accessible to water.

[1] V. Artemov, The Electrodynamics of Water and Ice, Springer, 2021

[2] A. Ryzhov et al., arXiv:2509.09462 (2026) – accepted in PRL

[3] V. Artemov et al., J. Phys. Chem. Lett., 11, 9, 3623 (2020)

[4] S. Melnik et al., J. Phys. Chem. Lett., 14, 29, 6572 (2023)

[5] V. Artemov et al., arXiv:2410.11983v4 (2026) – under review

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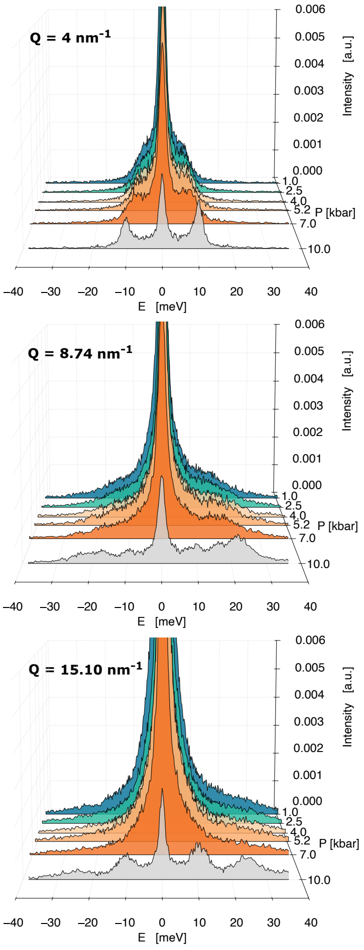
High pressure behavior of the low frequency mode of water

M. Rescigno[1], U.Ranieri[2], R. Gaal[3], L. Paolasini[4], F. Formisano[1], G. Radtke[5], P. Giura[5], and L. E. Bove[5, 6, 3]

[1]Institut Laue-Langevin, 71 Avenue des Martyrs, Cedex 9, Grenoble, France, [2]Centro de Fisica de Materiales (CFM-MPC), CSIC-UPV/EHU, Donostia/San Sebastian 20018, Spain, [3]Laboratory of Quantum Magnetism, Institute of Physics, Ecole Polytechnique F´ed´eerale de Lausanne, CH-1015 Lausanne, Switzerland, [4]European Synchrotron Radiation Facility, 71 Avenue des Martyrs, 38000 Grenoble, France, [5]Institut de Mineralogie, de Physique des Materiaux et de Cosmochimie (IMPMC), Sorbonne Universite, CNRS UMR 7590, MNHN, 4, place Jussieu, Paris, France, [6]Dipartimento di Fisica, Sapienza Universit`a di Roma, Piazzale Aldo Moro 5, 00185 Roma, Italy

The existence of a low-frequency (LF) and weakly-dispersing mode in the THz spectrum of liquid water is known since the seventy's but its microscopic origin is still debated [1]. First attributed to an optic transverse-like character [2] or, alternatively, to the result of a mode-mode interaction and symmetry avoided crossing [3], this mode is now more commonly associated with an acoustic transverse-like dynamics [4] at least at the lowest Qs [5]. In this talk I will present an investigation of the THz spectrum of water under pressure using high-resolution inelastic X-ray scattering (IXS) [6]. Measurements on H_2O and D_2O were performed at room temperature up to the ice VI crystalisation pressure at 1 GPa, spectra are shown in figure 1. The LF mode shows a weak sensitivity to pressure and remains overdamped throughout the explored range. Comparison with IXS measurements and ab initio simulations of crystalline Ice VI reveals a cluster of weakly dispersive modes in the same energy range, suggesting that the low-frequency mode in liquid water reflects a mixed character rather than being assigned to a purely transverse acoustic excitation. Our results provide new insight into the microscopic origin of water's anomalous THz dynamics under compression.



`rescigno@ill.fr`

[1] G. Ruocco and F. Sette, *The high-frequency dynamics of liquid water*, Journal of Physics: Condensed Matter 11, R259 (1999). [2] G. Ruocco et al, *Equivalence of* *and ice at mesoscopic wavelengths*, Nature 379, 521 (1996) [3] C. Petrillo et al, *High-resolution neutron scattering measurement of the dynamic structure factor of heavy water*, Phys. Rev. E 62, 3611 (2000) [4] E. Pontecorvo et al, *High-frequency longitudinal and transverse dynamics in water,* Phys. Rev. E 71, 011501 (2005) [5] A. De Francesco J. Chem. Phys. 158, 134509 (2023) [6] M. Rescigno et al, *High pressure behavior of the low frequency mode of water,* submitted

Figure 1: IXS spectra collected on ID28

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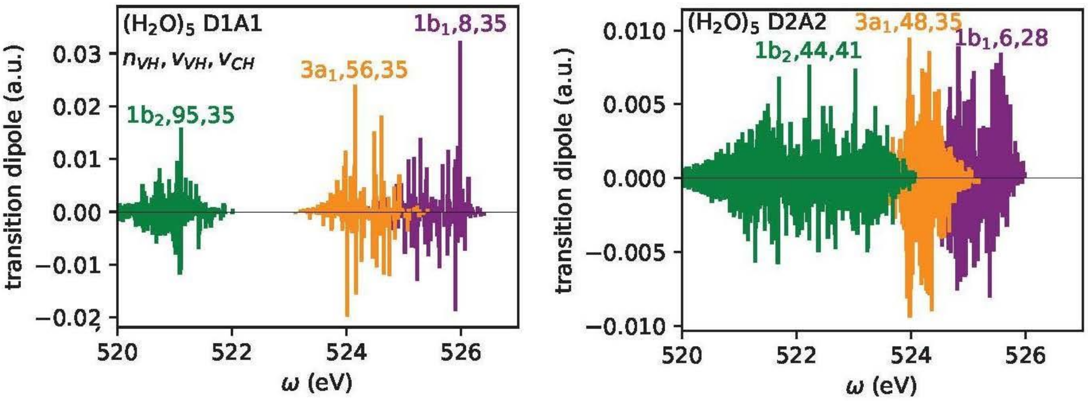
Interference Effects on the X-ray Emission Spectra of Liquid Water and Analysis of an Attosecond Pump-Probe Model

Félix Moncada, Thomas Fransson, Mathias P. Ljungberg, and Lars G. M. Pettersson

Department of Physics, Stockholm University, 109 61 Stockholm, Sweden

We report a detailed investigation of the importance of vibrational direct and interference effects in X-ray emission applied to water. We use the full Kramers-Heisenberg (KH) expression on a 2D grid with the two OH-stretches of a central water molecule as coordinates and solve for the relevant vibrational states providing direct and interference terms. For two pentamer models we show close agreement between high-level ADC(3) and TDDFT results and then apply to four larger 32-molecules clusters representing high- (HDL) and low-density liquid (LDL) and two intermediate structures. We find for HDL and LDL an initial split (without dynamics) of 0.6 eV, which is increased to 0.7 eV using the full KH expression, *i.e.* the observed split is dominated by the initial H-bonding. The importance of direct and interference contributions is different for HDL and LDL structures, where for HDL the full spectrum is well represented by either contribution, while for LDL the $3a_1$ is strongly enhanced in the direct spectrum while the $1b_1$ depends mainly on interference. In a recent attosecond X-ray pump/X-ray probe spectrum, only one $1b_1$ peak was observed together with a significantly increased intensity in the $3a_1$ region. We reassign the features as due to molecules in asymmetric H-bond situation ($1b_1$ peak) and molecules in tetrahedral H-bonding ($3a_1$ intensity) in this experiment where only direct terms contribute. To eliminate the need for precomputed potential energy surfaces we show that a semi-classical approximation to the KH formalism gives excellent agreement, including vibrational fine-structure, with the full KH spectra for the four 32-molecule clusters.



Computed KH amplitudes for the vibrational transitions involving each electronic final valence-hole state for asymmetric (D1A1) and tetrahedral (D2A2) pentamer models (violet: $1b_1$, orange: $3a_1$, green: $1b_2$).

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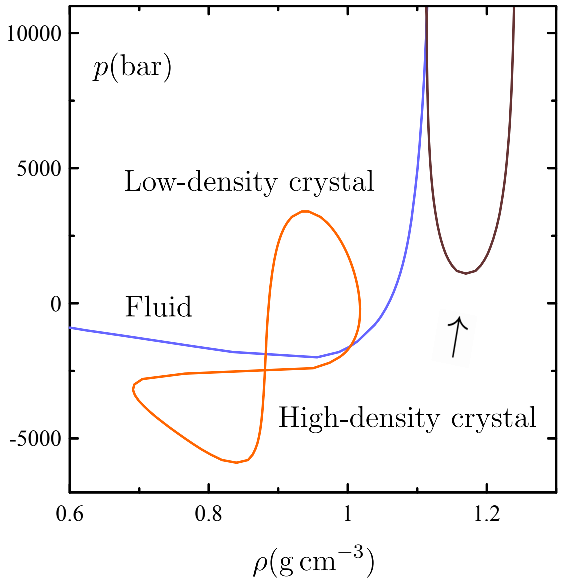
Theory of supercooled water

Jacobo Troncoso and Claudio A. Cerdeiriña
Instituto de Física, Computación e Ciencia Aeroespacial da Universidade de Vigo and Unidad MSMN Asociada al CSIC por el IQF Blas Cabrera, Ourense 32004, Spain

The "second-critical-point," "critical-point-free," and "singularity-free" scenarios for the unusual thermodynamics of supercooled water find theoretical support from an increasing number of analytically tractable models [1-4]. Nevertheless, all such models lack a description of the crystal, the freezing transition, and the associated metastable states, implying that the supercooled nature of the liquid phase is overlooked. Such an incomplete characterization prevents a full theoretical understanding.

Here we provide the desirable complete approach to the problem on the basis of a van der Waals-like theory consisting of Ising-like models studied at a mean-field level. In particular, on combining our recent prototypes for crystalline solids, freezing, and water's fluid phases, we manage to devise a five-state variant of the class capable to reproduce the second-critical-point and critical-point-free scenarios but also the stability-limit one early envisioned by Speedy and Angell [5].



Model's $T = 260$ K isotherm in the pressure-density p-ρ plane

[1] P. H. Poole, F. Sciortino, T. Grande, H. E. Stanley, and C. A. Angell, Phys. Rev. Lett. 1994, **73**, 1632.
[2] S. Sastry, P. G. Debenedetti, F. Sciortino, and H. E. Stanley, Phys. Rev. E 1996, **53**, 6144.
[3] P. Chitnelawong, F. Sciortino, and P. H. Poole, J. Chem. Phys. 2019, **150**, 234502.
[4] L. Verma and K. A. Dill, J. Chem. Theory Comp., 2025, **21**, 7755−7764 and references therein.
[5] R. J. Speedy, J. Phys. Chem. 1982, **86**, 982 and references therein.

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Hamiltonian limited valence model for liquid polyamorphism in water and other substances

Sergey V. Buldyrev

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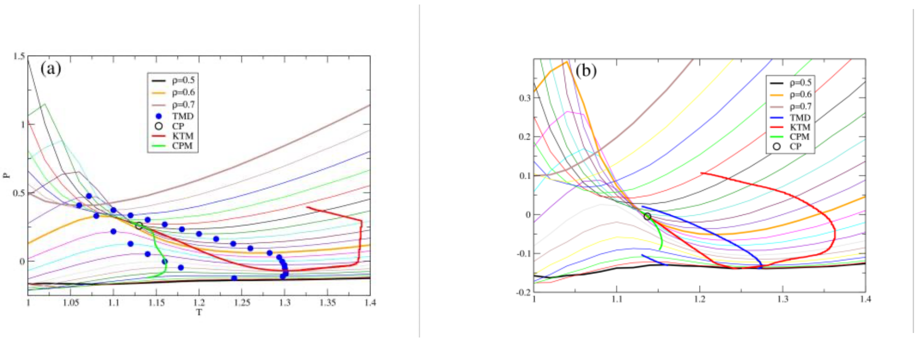
Department of Physics, Yeshiva University, New York NY 10033

Liquid–liquid phase transitions have been found experimentally or by computer simulations in many compounds such as water, hydrogen, sulfur, phosphorus, carbon, silica, and silicon. Limited valence model implemented via event-driven molecular dynamics algorithm provides a simple generic mechanism for the liquid–liquid phase transitions in all these diverse cases. Here [1], we introduce the limited valence model with a well-defined Hamiltonian, i.e., a unique algorithm by which the potential energy of the system of particles can be computed solely from the coordinates of the particles and is thus equivalent to a complex multi-body potential. We present several examples of the model which can be used to reproduce liquid–liquid phase transition in systems with maximum valence $z = 1$ (hydrogen), $z = 2$ (sulfur) and $z = 4$ (water), where z is the maximum number of bonds an atom is allowed to have. The limited valence model can be modified to forbid not only too large valences but also too low valences. The main focus of our study is water ($z = 4$) for which, based on the O-O radial distribution function, we find a set of parameters reproducing the phase diagram of water with a wide region of negative thermal expansion coefficient (density anomaly) extending into the metastable region of negative pressures.

[1] S.V. Buldyrev, Condensed Matter Physics **27**, 23601 (2024).
[2] Poole P. H., Saika-Voivod I., Sciortino F., J. Phys.: Condens. Matter., 2005, **17**, L431
[3] Sastry S., Debenedetti P. G., Sciortino F., Stanley H. E., Phys. Rev. E, 1996, **53**, 6144–6154



$P - T$ phase diagrams for $z = 4$ (water) with $w = 1.5$, $w_b = 1.1$, $\epsilon_b = -6$ and $\epsilon_z = 6$ for repulsive shoulder width $w_z = 1.34$ (a) and $w_z = 1.35$ (b). One can see the isochores crossing at the critical points surrounded by the region of the density anomaly as for the ST2 model of water. This region is separated by the TMD (temperature of maximum and minimum density) line connecting the points of minimum and maximum pressure at constant density. Also are shown the line of isothermal compressibility, κ_T maxima and minima (KTM) which crosses the TMD line at its vertical point and the constant pressure specific heat maxima (CPM) line (green) which coincides with the KTM line near the critical point. The TMD, KTM and CPM lines are obtained by the polynomial interpolation of the computed points on the isochores, obtained with steps $\Delta\rho = 0.01$ and $\Delta T = 0.01$. The low density isochores in (b) start to intersect with each other forming a liquid–gas spinodal, which becomes non-monotonic following the isochores with a minimum at the point of maximum density like in the IAPWS95 [68] equation of state of water extrapolated to the metastable region of negative pressures.

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WaterX - Program May 24 - May 29 2026 - La Maddalena (Italy)

time	Sunday May 24
18:30	**Welcome Cocktail**
21:00	**Opening Lecture: H. C. Allen**

time	Monday May 25
8:30	**Opening & Registration**
9:00	C. Salzmann
9:45	B. Journaux
10:15	G. Tobie
10:35	H. Kobayashi
10:55	I. Braslavsky
11:10	**Coffee Break**
11:40	F. Caupin
12:10	J. A. Troncoso
12:30	V. Molinero
12:50	F. Pabst
13:05	**Lunch**
14:30	A. Desmedt
15:00	L.-R. Fidler
15:20	L. Del Rosso
15:40	T. Poreba
16:00	K. Skrzyńska
16:15	**Excursion: Caprera Trail and beach**
19:30	**Sunset at Baia Trinita**

time	Tuesday May 26 - Chair. ....
6:00	**Sunrise Trail to Cala Napoletana #**
9:00	M. Bonn
9:45	C. Alba-Simionesco
10:15	D. Morineau
10:35	C. Vega
10:55	F. Leoni
11:10	**Coffee Break**
11:40	A. Ravasio
12:10	K. Mochizuki
12:30	U. Jones
12:45	K. Yamashita
13:00	**Lunch**
	Free Time Scuba Diving on demand **
16:00	T. Bartels-Rausch
16:30	C. Schran
17:00	X. Michaut
17:20	Z. Fakhoury
17:40	E. Sanz
18:00	**3-minute talk Poster presenters**
19:00	**Poster Session**

time	Wednesday May 27 Chair ....
9:00	H. Tanaka
9:45	F. Perakis
10:15	C. Stan
10:35	I. Saika-Voivod
10:55	R. Tyburski
11.10	**Coffe Break**
11:40	S. Xantheas
12:10	F. J. Blas
12:30	B. Chazallon
12:50	A. Stoporev
13:05	**Lunch**
14:30	N. Giovanbattista
15:00	F. Martelli
15:30	C. Pierleoni
15:50	A. Siciliano
16:05	**Coffee Break**
16:30	E. Adams
17:00	F. Turci
17:20	G. Graziano
17:40	C. Sun
18:00	I. Bako
18:20	**Walk to Punta Tegge for Sunset Apero ***

time	Thursday May 28- Chair ....
8:45	K. Koga
9:15	G. Franzese
9:45	A. Greco
10:05	**Boat trip to Maddalena Arcipelago ##**
20:00	**Social Dinner**

time	Friday May 29 Chair ....
9:00	M. Citroni
9:30	G. Sosso
09:50	D. V. Matyushov
10:10	V. Artemov
10:30	**Coffe Break**
11:00	M. Rescigno
11:15	L. Petterson
11:30	C. Cerdeiriña
11:50	S. V. Buldyrev
12:05	**Closing**

max 10 places available.

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

** Scuba-diving will be operated by Best Shark Diving Center upon request (Introductory lesson and excursions available: price TBD).

This activity is NOT included in the registration fee. It should cost about € 70/person (lunch included), a local fee of 5 € will be requested when entering the Parco dell'Arcipelago.