# Water Anomalies
# Origin and Implications

**10–12 Jun 2026**
**Stockholm**

**Location:**
Albano Building 2, Lecture room 17, Stockholm University, Albano campus, Norra Djurgården, Albanovägen 20, 114 19 Stockholm Go to map

**Wednesday June 10, 2026**

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|---|---|---|
| **8:30** | Registration | |
| **09:00** | **F. Perakis, A. Nilsson** | Welcome, Opening remarks |
| **09:15** | **F. Sciortino** | Plenary talk: Overview and some recent results |
| **10:00** | **P. Gallo** | Water and "The Others" |
| **10:30** | Coffee break | |
| **11:00** | **M. Havenith** | Caught in the act: Time resolved THz spectroscopy puts the spotlight on the role of the solvent into photochemical reactions |
| **11:30** | **F. Paesani** | A Data-Driven Many-Body Perspective on Aqueous Systems Across Phases |
| **12:00** | Lunch break | (Proviant Albano, hus 2) |
| **13:30** | **M. Anisimov** | Interconversion of two states: generic description of fluid polyamorphism |
| **14:00** | **G. Kontogeorgis** | Water thermodynamics - from a (chemical) engineering point of view |
| **14:30** | **C. Vega** | Simulating electrolytes with simple models |
| **15:00** | Coffee Break | |
| **15:30** | **L. Pettersson** | Searching for LDL templates in water |
| **16:00** | **S. Xantheas** | Liquid water is markedly different than liquid $H_2X$ (X = S, Se, Te) |
| **16:30** | **R. Signorell** | Chemistry in aqueous droplets |
| **17:30** | Welcome reception and poster session (Proviant Albano, hus 2) | |

**Thursday June 11, 2026**

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| **09:00** | **P. Debenedetti** | Computational Studies of Water Glasses |
| **09:30** | **N. Giovambattista** | Nuclear Quantum Effects in Water and Biomolecules |
| **10:00** | **N. E. Levinger** | The trouble with water. Exploring how cryoprotecting agents mitigate effects of low temperature on plant cells and tissue |
| **10:30** | Coffee break | |
| **11:00** | **K. H. Kim** | Unveiling the Origin of Water’s Anomalous Properties with X-ray Lasers |
| **11:30** | **S. Saito** | Microscopic Origins of Water Anomalies to Dynamic Slowdown |
| **12:00** | Lunch break | (Proviant Albano, hus 2) |
| **13:30** | **G. Kimmel** | Dynamics in supercooled water |
| **14:00** | **A. Hassanali** | Glassy Arrest in Supercooled Water |
| **14:30** | **K. Amann-Winkel** | X-ray scattering on amorphous ices: key to water's hidden states |
| **15:00** | **S. Sastry** | Out-of-Equilibrium Potential Energy Landscape Equation of State of Shear-driven Amorphous Ice |
| **15:30** | Coffee break | |
| **16:00** | **E. Backus** | Temperature-dependent vibrational energy relaxation at the air–water interface |
| **16:30** | **M. Bonn** | Confined and Interfacial Water: Insights from Surface Vibrational Spectroscopy |
| **17:00** | **M. Beye** | Non-linear X-ray approaches |
| **17:30** | **V. Kocherbitov** | Coupling between structural evolution and glass transition in supercooled water |

**Friday June 12, 2026**

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| **09:00** | **P. Poole** | Liquid-Liquid Phase Transition in Simulated Supercooled Water Nanodroplets |
| **09:30** | **B. Wyslouzil** | Freezing nanodroplets: Probing water's phase transitions under extreme conditions |
| **10:00** | **P. Singh** | The interfacial molecular structure and electrostatics of nanodroplets |
| **10:30** | Coffee break | |
| **11:00** | **J. Sellberg** | Fluctuation x-ray scattering of micron-sized water droplets |
| **11:30** | **Y. Harada** | Size and Charge Characteristics of Pure-Water Nanodroplets Generated by Collision Nebulization |
| **12:00** | Lunch break | (Proviant Albano, hus 2) |
| **13:30** | **L. Bove** | How plastic water is? |
| **14:00** | **H. Tanaka** | Origin of Water’s Surface-Tension Anomaly and Surface-Induced Crystallization |
| **14:30** | **L. Xu** | Ice Crystallization and premelting in low dimensions: an atomic-scale view |
| **15:00** | **C. Salzmann** | Heterogeneous Nucleation and Interfacial Water Structure: From Atmospheric Microplastics to Heat-Battery Materials |
| **16:00** | Excursion and Dinner at Fjäderholmarna<br>Restaurant: Fjäderholmarnas Krog<br>Address: Stora Fjäderholmen, 100 05 Stockholm<br><br>17:30 The boat departs from Nybroviken<br>(Boat operator: Strömma Address: Strandvägen – Pier Area 13)<br><br>18:00 Welcome drink (one glass of sparkling wine will be served upon arrival)<br><br>18:20 Dinner is served with 2 glasses of wine<br><br>21:00 Boat back to Nybroviken | |

# Abstracts

**Katrin Amann-Winkel,** Johannes Gutenberg University Mainz
***X-ray scattering on amorphous ices: key to water's hidden states***
Amorphous states of water play an important role in the ongoing debate about the origin of water´s anomalies. Since the discovery of two distinct amorphous states of ice with different density (high- and low-density amorphous ice, HDA and LDA) it has been discussed whether and how this phenomenon of polyamorphism at high pressure is connected to the occurrence of two distinct liquid phases (HDL and LDL). While HDA can only be prepared by pressure induced amorphization, LDA can also be made by vapor deposition, then called amorphous solid water (ASW). X-ray scattering experiments on differently prepared amorphous ices are of major importance for a deeper understanding of water´s phase diagram. In my talk, I will give an overview about recent experiments on compressed water and vapor deposited amorphous ice, using X-ray photon correlation spectroscopy (XPCS) as well as time-resolved diffraction.

**Mikhail Anisimov ,** University of Maryland, College Park.
***Interconversion of two states: generic description of fluid polyamorphism***
Liquid-liquid phase transition in deeply supercooled water is just a most fascinating example of fluid polyamorphism, the existence of two or more fluid-fluid transitions and the possibility of multiple fluid-fluid critical points in a single-component substance. In my presentation I will explain the similarity and the difference between nondegenerate fluid polyamorphism, such as in water, and degenerate fluid polyamorphism in helium-4. The degenerate polyamorphism is caused by degenerate interconversion of molecular states, in which the enthalpy of interconversion is zero and the fraction of interconversion changes only in the ordered state with the change of the order parameter. The difference between these two kinds of interconversion is the reason for fundamentally different phase behavior of supercooled water and helium-4. Other substances exhibiting nondegenerate fluid polyamorphism, such as hydrogen and sulfur are also discussed.

**Martin Beye,** Stockholm University
***Non-linear X-ray approaches***
The short wavelength of X-rays gives unique access to atomic lengthscales, while their energy tunability can be used to separate different chemical species. Non-linear methods can have special selection rules, like for example surface selectivity, or can generate very specific signals often in background-free geometries. Despite small conversion efficiencies, such signals can thus be easily recorded. The combination of the features of X-rays with non-linear methods is in its infancy, but holds interesting promises for future research. I will give an overview of the state of the field in general and highlight some applications that might open future perspectives in the research on water.

**Mischa Bonn,** Max-Planck Institute for Polymer Research
***Confined and Interfacial Water: Insights from Surface Vibrational Spectroscopy***
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 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 used in nanofluidic technology, such as hexagonal boron nitride,

acquire a spontaneous surface charge upon contact with water [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, but in remarkably good agreement with simple hundred-year-old predictions from Debye [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).

**Livia Bove,** CNRS & Università La Sapienza
***How plastic water is?***
Over the past decade, computer simulations [1-3] have predicted the existence of a novel phase of water, termed "plastic ice," expected to emerge along the melting line between liquid water and ice VII, as well as in water mixtures under extreme pressure–temperature (p–T) conditions. In this phase, water molecules maintain long-range crystalline order while retaining orientational freedom, giving rise to a hybrid solid–liquid state. While plasticity is well documented in crystals of globular molecules such as methane, its occurrence in water ice is far from trivial. Our recent high-pressure quasielastic neutron scattering (HP-QENS) experiments have revealed varying degrees of plasticity across a broad range of aqueous systems, including high-pressure ice [4] phases, water–ammonia solid solutions [5], salty ices [6], methane- and hydrogen-filled ices [7-9] , and confined amorphous ice [10]. In this talk, I will discuss how plasticity emerges across diverse chemical environments and p–T conditions and its connection to the "glassy" dynamics of water.
[1] J. L. Aragones and C. Vega, Journal of Chemical Physics 130, 244504 (2009);
[2] K. Himoto, M. Matsumoto and H. Tanaka, Phys. Chem. Chem. Phys., 13, 19876–19881 (2011);
[3] Hernandez,J.-A., Caracas, R.: Physical Review Letters 117(13), 135503 (2020) ;
[4] Rescigno, M., Toffano, A., Ranieri, U. et al. Observation of Plastic Ice VII by Quasi-Elastic Neutron Scattering, Nature 640 (8059), 662–667 (2025). DOI:10.1038/s41586-025-08750-4;
[5] H. Zhang, et al., The Journal of Physical Chemistry Letters 14(9) 2301 (2023);
[6] A. Nichols et al., Earth and Planetary Science Letters submitted (2025);
[7] U. Ranieri et al., PNAS 120 52 (2023);
[8] Di Cataldo et al., Phys. Rev. Letters. 133 23 (2024);
[9] L. Renaud, et al., Proc. Natl.Acad. Sci. USA (2026). DOI: 10.1073/pnas.2526369123;
[10] M. Rescigno et al., J.Phys. Chem. B (2023) 127 (20), 4570-4576.

**Pablo Debenedetti,** Princeton University
***Computational Studies of Water Glasses***
I will present results from three ongoing computational projects, with water glasses as the common theme. First, I will discuss some aspects of the interesting and largely unexplored physics that arises in supercooled water due to the proximity of the liquid-liquid critical point and the glass transition loci [1,2]. Computer simulations show clear signatures of critical behavior in glasses formed near water's second critical point. I will then present results on the energy landscape of the machine-learned DP-MBpol model [3]. The resulting equation of state predicts a liquid-liquid critical point in very good agreement with recent estimates [4]. This shows that metastable criticality is encoded in this model, adding to similar evidence for realistic classical models [5-7]. Finally, I will discuss a computational study of cryogenic electron microscopy (cryo-EM), a technique that has enabled near-atomic resolution structure determination of biomolecules, and in which sample suspension in a glassy water matrix plays a central role. Using a combination of molecular dynamics, Markov State modeling and thermodynamic inference, we quantify the extent to which vitrification alters the TrpCage mini-protein's conformational ensemble relative to the starting equilibrium distribution
[1] Gartner et al., Nature Comm., 12, 3398 (2021).

[2] Szukalo et al., PNAS, 122, e2509609122 (2025).
[3] Szukalo et al., PNAS, 123, e2534303123 (2026).
[4] Sciortino et al., Nat. Phys., 21, 1 (2025).
[5] Handle and Sciortino, J. Chem. Phys., 148, 134505 (2018).
[6] Handle et al., J. Chem. Phys., 150, 244506 (2019).
[7] Eltareb et al., J. Chem. Phys., 160, 154510 (2024).
[8] Clark et al., bioRxiv 2026.04.21.72011V1 (2026).

**Nancy E. Levinger,** Colorado State University
***The trouble with water. Exploring how cryoprotecting agents mitigate effects of low temperature on plant cells and tissue***
The basic but unusual characteristics of water make it the substance of life. And yet, the high water content of living organisms makes them vulnerable when temperatures drop and crystalline ice forms. Cryopreservation of live cells and tissue is used to maintain sample viability at low temperatures. To be effective, cryopreservation relies on the addition of cryoprotecting agents, that is, molecules that mitigate damage from ice formation. The Levinger group has pioneered methods to measure how traditional cryoprotectants interact with plant cells and tissue. Via CARS and brightfield microscopy, we measure the permeation and flow of water, and the components of a common plant cryoprotectant formulation, in and out of rice callus cells and peppermint shoot tips. All the molecules measured, i.e., water/D2O, DMSO, ethylene glycol, glycerol and sucrose, pass quickly and efficiently into and out of plant material, sometimes concentrating locally within the plant material. We use this information to understand how these materials work to protect samples in cryostorage.

**Paola Gallo,** University Roma Tre
***Water and "The Others"***
Water is a complex system where computer science plays a crucial role. Classic computer molecular dynamics simulations in particular are pivotal to study the behavior of water and aqueous solutions under extreme conditions. Especially in the supercooled region that is to date only partially accessed by experiments. I will illustrate recent studies on water in solutions where computer simulations show results in line with experiments and produce further results in regions of the phase diagram not explored so far by experiments. I will focus on thermodynamics, slow dynamics and structure upon cooling for water in solutions with different solutes and on the differences of behaviours with respect to the bulk. The results that I will discuss will show to what extent water anomalies matter when water is in solutions that are of interest for outer planets science, in particular for the research about water on Mars and for water on the icy moons of Jupiter, and for cryobiology [1,2].
[1] L. Perin and P. Gallo, The effect of the cryoprotectant dimethyl sulfoxide on water upon supercooling: A molecular dynamics study The Journal of Chemical Physics 163, 214501 (2025).
[2] P. La Francesca and P. Gallo, Molecular Dynamics Simulations of Supercooled Aqueous Solutions of Calcium Perchlorate: Thermodynamics and Structure of Martian Solutes in TIP4P/2005 Water The Journal of Physical Chemistry B 129, 8776 (2025).

**Nicolas Giovambattista,** Brooklyn College
***Nuclear Quantum Effects in Water and Biomolecules***
Nuclear quantum effects (NQE), arising mainly from the H atoms delocalization, modulate hydrogen bonding in water and can therefore alter its structural, dynamical, and thermodynamic properties. In this talk, we will discuss path-integral computer simulations results quantifying the impact of NQE on: (i) the phase behavior of supercooled water, with emphasis on the liquid–liquid critical point (LLCP) location; and (ii) the temperature- and pressure-dependent behavior of a small peptide, α helical polyalanine. For supercooled water, NQE produce a systematic shift of the LLCP and overall phase diagram toward lower temperatures and pressures. In contrast, for the model peptide studied, our

simulations at low and intermediate pressures indicate that NQE exert only a limited influence on polyalanine properties.

**Lars G. M. Pettersson,** Stockholm University
***Searching for LDL templates in water***
In the single-phase region beyond a critical point there are fluctuations between remnants of the pure phases. For water this would relate to HDL and LDL, but what are these structures? Here, I will discuss the FCM/GAP force field and how we use a machine-learned version to investigate the possible existence of specific dodecahedral templates that might form on some time-scale.

**Christoph G. Salzmann,** University College London
***Heterogeneous Nucleation and Interfacial Water Structure: From Atmospheric Microplastics to Heat-Battery Materials***
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 $CaCl \cdot 2H O$ 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

**Yoshihisa Harada,** University of Tokyo
***Size and Charge Characteristics of Pure-Water Nanodroplets Generated by Collision Nebulization***
The generation of pure-water nanodroplets and the characterization of their size and charge states are important for understanding nanoscale gas–water interfacial dynamics. In this study, we investigated a pure-water nanodroplet system generated by collision nebulization. The size and charge characteristics of gas-phase particles were analyzed using ELPI/SMPS, while nanoparticle tracking analysis (NTA) was employed to examine the processes of generation and transport. Our results show that this system produces nanodroplets with characteristic size distributions and charge properties. Furthermore, two distinct types of structures were identified during transport: clustered structures and more sparsely distributed structures. These observations suggest that the pure-water nanodroplet system does not remain in a simple equilibrium state, but instead undergoes dynamic

evolution. This study thus provides new experimental insight into the formation of pure-water nanodroplets, their size and charge characteristics, and the interfacial structures associated with transport.

**Ali Hassanali,** The Abdus Salam International Center for Theoretical Physics
***Two Liquids in One - Or is One Getting Glassier?***
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 may instead originate from the onset of glassy dynamics. Specifically, we find that the fluctuations previously associated with an LLT 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.

**Martina Havenith,** Department of Physical Chemistry II, Ruhr University Bochum, Germany
***Caught in the act: Time resolved THz spectroscopy puts the spotlight on the role of the solvent into photochemical reactions***
The development of time-resolved and surface-sensitive spectroscopies in the UV, optical, and IR frequency ranges has impacted our understanding of chemical reactions. Probing intermediates and transition states can now be probed experimentally, and in doing so, provide new perspectives on reaction pathways and dynamics. These techniques have so far mainly focused on solutes, reactants, and products. Our goal is to put the spotlight on the solvent and visualize the correlated electron and solvent dynamics in electrocatalysis and biological processes. While optical and IR spectroscopy can report on electronic states, the Stokes shift, and intramolecular modes, they provide less information on the non-covalent and intermolecular interactions involved. We use THz spectroscopy as the most sensitive tool to probe intermolecular interactions, such as hydrogen bonding and local solvation motifs [1]. Most notable changes in these can be directly correlated to changes in solvation entropy and enthalpy, e.g., changes in free energy, upon desolvation and resolvation [2]. Unlike conventional calorimetry, "THz calorimetry", which is based on spectroscopic observables, can be applied to inhomogeneous samples and can monitor the solvent response and the propagation of vibrational energy upon photoexcitation on a ps time scale by optical pump terahertz probe (OPTP) [3,4].
[1] K. Mauelshagen, P. Schienbein, I. Kolling, G. Schwaab, D. Marx, M. Havenith, Random encounters dominate water-water interactions at supercritical conditions, Sci. Adv. 11, eadp8614 (2025).
[2] S. Pezzotti, W. Chen, F. Novelli, X. Yu, C. Hoberg, M. Havenith, Terahertz calorimetry spotlights the role of water in biological processes, Nat. Rev. Chem. 9, 481–494 (2025).
[3] S.S. Nalige, P. Galonska, P. Kelich, L. Sistemich, C. Herrmann, L. Vukovic, S. Kruss, M. Havenith, Fluorescence changes in carbon nanotube sensors correlate with THz absorption of hydration. Nat. Commun. 15, 6770 (2024).
[4] F. Novelli, K. Chen, A. Buchmann, T. Ockelmann, C. Hoberg, T. Head-Gordon, M. Havenith, The birth and evolution of solvated electrons in the water, PNAS 120, e2216480120 (2023).

**Ellen H. G. Backus,** University of Vienna
***Temperature-dependent vibrational energy relaxation at the air–water interface***
The interplay of water with other media is always mediated by an interface, which ultimately regulates interactions and energy flow. Vibrational sum-frequency generation (vSFG) spectroscopy provides structural and dynamic information on water molecules at interfaces. It has revealed, for instance, the

presence of the hydrogen bonded and free OH groups at the air–water interface. Furthermore, water properties are temperature dependent (such as density, viscosity, static dielectric constant, etc.) and also at the interface (e.g., surface tension). Consequently, temperature determines the behavior of water at interfaces, making it a critical factor in interfacial phenomena. Here, using temperature-dependent, time-resolved vSFG, we focus on the vibrational energy relaxation dynamics of interfacial heavy water (D2O). We reveal that while the relaxation timescale for hydrogen-bonded OD stretch modes is temperature-independent, the lifetime of the free OD stretch mode decreases with increasing temperature. Our data, supported by simulations, suggest that both intramolecular energy transfer and rotational reorientation mechanisms jointly contribute to the energy relaxation process of the free OD, with temperature influencing these mechanisms differently.

**Kyung Hwan Kim,** POSTECH
***Unveiling the Origin of Water's Anomalous Properties with X-ray Lasers***
Water is the most important material for our life on Earth and plays an essential role in countless physical, chemical, and biological processes. Despite its importance, the microscopic origin of water's anomalous properties has remained one of the most enduring questions and the issue has been intensely debated for decades because the relevant supercooled states are extremely difficult to probe experimentally before water crystallizes. In recent years, we have opened a new route to directly access these elusive states by utilizing ultrafast X-ray techniques. In this talk, I will present our recent experimental results on the origin of water's thermodynamic [1,2,3] and dynamic [4] anomalies.
[1] S. You†, M. L.Parada†, K. Nam, A. Karina, S. Lee, M. Shin, C. Yang, Y. Han, S. Jeong, K. Park, K. Kim, M. Ki, R. Tyburski, I. Andronis, K. Ralf, J. H. Lee, I. Eom, M. Kim, R. Ma, D. Jang, F. Perakis, P. H. Poole, K. Amann-Winkel, K. H. Kim* and A. Nilsson*, Science, Accepted for publication.
[2] K. H. Kim†, K. Amann-Winkel†, N.Giovambattista, A. Späh, F. Perakis, H. Pathak, M. L. Parada, C. Yang, D.Mariedahl, T. Eklund, T. J. Lane, S. You, S. Jeong, M. Weston, J. H. Lee, I. Eom, M. Kim, J. Park, S. H. Chun, P. H. Poole, and A. Nilsson*, Science, 370, 978-982 (2020).
[3] K. H. Kim†, A. Späh†, H. Pathak, F. Perakis, D. Mariedahl, K.Amann-Winkel, J. A. Sellberg, J. H. Lee, S. Kim, J. Park, K. H. Nam, T. Katayama, and A. Nilsson*, Science, 358, 1589-1593 (2017). 4. Tyburski†, M. Shin†, S. You, K. Nam, M. Soldemo, A. Girelli, M. Bin, S. Lee, I. Andronis, Y. Han, S. Jeong, R. A. Oggenfuss, R. Mankowsky, D. Babich, X. Liu, S. Zerdane, T. Katayama, H. Lemke, F. Perakis, A. Nilsson*, and K. H. Kim, Nat. Phys., 22, 21-26 (2026).

**Greg Kimmel,** Northwest National Laboratory
***Dynamics in supercooled water***
To avoid crystallization, experiments on deeply supercooled water often employ rapid changes in temperature and/or pressure. How closely such experiments track the "equilibrium" properties of supercooled water is a topic of ongoing debate. To help address this issue, we used a pulsed laser heating method to investigate diffusion in water for temperatures between 250 K and 190 K. Over that temperature range, the diffusion decreases by approximately 5 orders of magnitude, and switches from super-Arrhenius to (apparently) Arrhenius behavior. Interestingly, the diffusion matches earlier predictions that were based on the thermodynamics of water outside of “No Man’s Land” and the Adam-Gibbs model, which relates the dynamics of supercooled liquids to their configurational entropy. The observations suggest that even at very high heating and cooling rates, the resulting non-equilibrium dynamics are similar to the dynamics expected at equilibrium.

**Vitaly Kocherbitov,** Malmö University
***Coupling between structural evolution and glass transition in supercooled water***
Water exhibits unique structural, thermodynamic, and dynamic anomalies, particularly in supercooled states where structural evolution between high- and low-density liquid environments occurs alongside kinetic arrest. Here we present molecular dynamics simulations of water in a broad range of cooling and heating rates to investigate equilibrium and nonequilibrium behavior. Above ~220 K, properties are scan-rate independent, indicating equilibrium, while below this temperature kinetic effects

dominate, reflecting glassy dynamics. In the liquid regime, the temperature dependence of viscosity reveals two relaxation mechanisms with distinct activation energies. The rapid slowing down of the lower-temperature mechanism leads to the onset of the glass transition. We find that the simulated glass transition occurs at the same temperature as the heat-capacity maximum associated with the gradual structural evolution between high- and low-density liquid environments. By integrating a two-state thermodynamic model with the Tool–Narayanaswamy–Moynihan glass-transition framework, we separate equilibrium anomalies from kinetic glass-transition effects. This combined approach provides a consistent description of water's coupled thermodynamic and dynamic behavior across a broad temperature range, clarifying the origin of its low-temperature anomalies.

**Georgios Kontogeorgis,** Technical University of Denmark
***Water thermodynamics - from a (chemical) engineering point of view***
Water is a very important molecule in all aspects and numerous engineering applications are closely related to water's thermodynamic properties. The interactions of water with electrolytes and in other systems are also very crucial. Since about 1990's a new family of thermodynamic models (SAFT) has appeared which are particularly useful for complex hydrogen bonding molecules. These models have been partially successful for water as well, especially phase behavior, but cannot describe water's anomalous properties. Incorporating the so-called two state theory in these advanced models appears to be a promising way forward towards describing a wider range of water properties. In this talk we will present historical and recent developments in water thermodynamics which can be of relevance to engineering applications.

**Francesco Paesani,** University of California
***A Data-Driven Many-Body Perspective on Aqueous Systems Across Phases***
Achieving chemical accuracy in molecular simulations of aqueous systems has remained elusive due to the interplay of many-body interactions and nuclear quantum effects. In this talk, I will present a unified data-driven many-body (DD-MB) formalism that enables realistic simulations of water and aqueous systems from small gas-phase clusters to bulk solutions and interfaces. By combining physics-based representations with machine-learned components trained on coupled-cluster reference data, our DD-MB potential energy functions, including MB-pol and its extensions, accurately reproduce structural, thermodynamic, and spectroscopic properties across phases, while providing a consistent molecular-level description of aqueous environments. I will discuss how the DD-MB formalism enables predictive simulations of complex phenomena, including the behavior of supercooled water and the emergence of a liquid–liquid critical point, and outline ongoing efforts to extend the DD-MB formalism to increasingly complex molecular systems.

**Peter Poole,** St. Francis Xavier University
***Liquid-Liquid Phase Transition in Simulated Supercooled Water Nanodroplets***
Using simulations, we demonstrate how a liquid-liquid phase transition (LLPT) manifests in supercooled water nanodroplets [1]. Selecting an interaction potential for which a LLPT occurs in the bulk liquid, we conduct simulations of supercooled water nanodroplets having between 1000 and 80000 molecules. We show that as the droplet size decreases, the Laplace pressure grows large enough to drive the droplets through the transition from the low-density to the high-density liquid phase, and that all droplets in this size range are large enough to have cores exhibiting the structure and properties of bulk water. To guide experiments, we estimate the range of values for the critical pressure of the LLPT in real water that can be observed using nanodroplets, and propose structural and dynamical measures by which the LLPT in nanodroplets can be detected.
[1] S.M.A. Malek, F.Sciortino, P.H. Poole, and I. Saika-Voivod, Phys. Rev. Lett. 134, 138001 (2025).

**Poonam Singh,** EPFL
***The interfacial molecular structure and electrostatics of nanodroplets***

Water is the liquid for life. It is intimately linked to our well-being. Without water, cell membranes cannot function. Charges and charged groups cannot be dissolved, self-assembly cannot occur, and proteins cannot fold. Because of the complexity of liquid water and aqueous interfaces, the relationship between the unique properties of water and its molecular structure has not been solved. This is especially true for nanoscale interfaces, on which the molecular level structure of water is hard to access. Using a combination of nonlinear optical light scattering and imaging techniques we investigated the molecular interfacial structure (water and substrate) in contact with hydrophobic nanoscale oil droplets in water and water in oil [1,2]. The surface potential, charge, and interfacial molecular structure was measured using the optical response of the interface. We show that all these metrics are identical at neutral and mildly basic pH (pH 7 and 11). The negative charge on the droplet surface is due to charge transfer [1] from and within water, and anisotropic gradients in the fluctuating polarization induced by the electric field [3]. Electrophoretic flow is induced by a combination of charge transfer / polarization which couples to an external electric field. The pH dependence of electrophoretic flow is caused by the Grotthuss mechanism, which reduces the resistance of bulk water to charge flow. This general mechanism deeply impacts a plethora of processes in biology, chemistry, and nanotechnology. It provides an explanation of how pH influences hydrodynamic phenomena and the limitations of classical continuum theory currently used to rationalize these effects.

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**Shinji Saito,** Institute for Molecular Science

***Microscopic Origins of Water Anomalies to Dynamic Slowdown***

Water is the most ubiquitous liquid and exhibits a variety of anomalies not observed in other substances. These anomalies become increasingly pronounced in the supercooled regime, making the understanding of deeply supercooled water a fundamental challenge. Experimentally, this regime remains elusive due to rapid crystallization, while computationally, the exponential growth of relaxation times poses a significant hurdle for standard molecular dynamics (MD) simulations. More generally, the dramatic dynamical slowdown upon cooling is a universal feature of glass-forming liquids, yet its temperature dependence—ranging from “strong” to “fragile” behavior—varies significantly across materials. In this presentation, we first discuss structural features of supercooled water that are thought to underpin its thermodynamic anomalies. We then introduce a theoretical framework based on dynamic disorder to elucidate the microscopic origin of the dynamic slowdown in supercooled liquids. This framework provides a unified, microscopic perspective on slow dynamics in water and in a wide range of liquids.

**Srikanth Sastry,** Jawaharlal Nehru Centre for Adv. Sc. Res.

***Out-of-Equilibrium Potential Energy Landscape Equation of State of Shear-driven Amorphous Ice***

We investigate shear-driven amorphous ice, motivated by the recent experimental discovery of Medium Density Amorphous (MDA) ice, and computational investigations that seek to understand MDA in terms of shear-driven non-equilibrium steady states. We perform a computational investigation of shear-driven amorphous ice (SDA), employing the TIP4P/2005 model, and address the question of whether their properties can be captured by approaches to the describe the thermodynamics of such steady states. Specifically, we explore whether the out-of-equilibrium (OOE) extensions of the equation of state (EOS) of low temperature liquids and glasses, evaluated within the framework of the potential energy landscape (PEL) approach, is capable of describing faithfully the

properties of SDA. The out-of-equilibrium equation of state relies on identifying an effective temperature that characterizes the structural state of the steady states, and evaluation of the vibrational free energy at the imposed bath temperature. We present results concerning the thermodynamics of SDA from simulations and compare it with the OOE equation of state results. We also compare the structure with expectations from the effective temperature description. In particular, we compare average descriptions of the shape of the basins, obtained from the vibrational frequencies. We further investigate the possible physical origin of the energy landscape explored in the steady states, in terms of the imposed shear rate and relevant structural relaxation times. We discuss the extent to which the OOE EOS approach provides a reasonable description of the steady states under shear, and the nature of the deviations.
* Work done in collaboration with Himangsu Bhaumik, Prashanti Jami, Andreas Neophytu, Francesco Sciortino and Vivek Sudhir.

**Francesco Sciortino,** Sapienza Universita' di Roma
***Some recent results***
Abstract: I will report some recent results on the behavior of water close to the liquid-liquid critical point. More specifically, I will discuss the dynamics of conserved and non-conserved order parameters, in the proximity of the liquid-liquid critical point. I will analyze how density and structural order parameters de-correlate over distances comparable to the correlation length, under conditions where the latter is governed by proximity to the liquid--liquid critical point (LLCP). Addressing this problem demands extremely large system sizes and very long simulation times at state points very close to the LLCP, where critical fluctuations are significant.

**Jonas Sellberg,** KTH
***Fluctuation x-ray scattering of micron-sized water droplets***
Abstract: Water is one of the most ubiquitous and vital substances for our survival and is thus also one of the most well-studied samples in fundamental research. We have over the past decade used x-ray scattering at x-ray free-electron lasers (XFELs) to study the structure of water upon deep supercooling and the structure of ice during subsequent crystallization. This is achieved by evaporative cooling of micron-sized water droplets in vacuo down to ~230 K and intersecting the droplets with the ultrabright, coherent x-ray beam. The initial experiments revealed a continuous increase in tetrahedral coordination among the structural motifs in the liquid upon deep supercooling. Simultaneously, crystallization increases rapidly, suggesting that the barrier to form an ice nucleus of critical size is quickly reduced at these temperatures. Herein, we present a method to use fluctuation x-ray scattering to obtain 3D structural information about the growing crystal in solution as well as the precursor liquid preceding nucleation. By calculating the pair-angle distance function it is possible to reveal structural motifs that aid or frustrate spontaneous nucleation and subsequent crystal growth. We present preliminary results using this technique from an experiment performed at the SPB/SFX instrument at the European XFEL, during which 76 million diffraction patterns of water and ice were recorded for 2–10 μm water droplets at various distances from the nozzle. (Acknowledgement: This work was funded by Swedish Research Council (Starting Grant No. 2017-05128) and Göran Gustafsson Foundation (Grant No. 1808)).

**Ruth Signorell,** ETH Zurich
***Chemistry in aqueous droplets***
The influence of acidity on bulk phase chemistry is well established. For chemical reactions that take place in droplets, its influence is less clear and less well studied. For example, the long-debated question of air-water interfacial acidity becomes criticial in droplets due to their extremely high surface-to-volume ratio, while it is negligible in bulk phase reactions. In my presentation, I will discuss specific examples of unexpected chemical reactions in droplets where the acidity is a key factor. This ranges from our recent observation of acid-catalyzed urea formation from carbon dioxide and ammonia in aqueous droplets [1] to challenges related to the distribution of acids and bases between

the gas and droplet phase. Our experiments utilize the advantages of single-droplet studies. We combine immobilization of single aerosol droplets in optical traps with sensitive in-trap detection methods, such as Raman and photoacoustic spectroscopy [1,2].
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**Hajime Tanaka,** University of Tokyo
***Origin of Water's Surface-Tension Anomaly and Surface-Induced Crystallization***
Water's surface tension shows an unusual nonlinear temperature dependence, including a reentrant increase in the supercooled regime. In this talk, I will present molecular dynamics simulations that reveal a structural origin of this anomaly by connecting microscopic ordering to macroscopic interfacial behavior. We demonstrate that surface tension is governed by the interplay between two local motifs: ρ-states, characterized by O–H alignment under surface symmetry breaking, and tetrahedral S-states, which are stabilized in the subsurface by negative pressure. At intermediate temperatures, the anisotropy of the ρ-states saturates while the S-states remain weakly anisotropic, leading to a slower increase in surface tension. Under deeper supercooling, the S-states acquire orientational order, which amplifies interfacial anisotropy and produces the reentrant rise in γ. This picture explains the inflection points in γ(T), clarifies the structural origin of water's surface-tension anomaly, and shows how surface ordering can enhance ice nucleation. The results have broader implications for nucleation, cryopreservation, ferroelectric-like ordering, and other network-forming liquids.

**Carlos Vega,** Complutense University of Madrid
***Simulating electrolytes with simple models***
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 present the development of the Madrid-2019 force field, which utilizes the TIP4P/2005 model for water and scaled charges for the ions. The force field includes parameters for the following cations: Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba, ammonium, hydronium; and for the anions: F, Cl, Br, I, sulfate, nitrate, perchlorate, and hydroxide [1-6]. As such, the force field can describe up to 88 different salts. We will present results for properties such as densities, structure, viscosities, diffusion coefficients, freezing point depression, and the density maximum. The choice of scaled charge values will also be discussed, as it is not possible to reproduce all properties with a single scaled charge [7]. Finally, we will address the transferability issue to the TIP4P/ice model of water and provide some results for a transition metal, such as Fe. [8]
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**Barbaba Wyslouzil,** Ohio State University
***Freezing nanodroplets: Probing water's phase transitions under extreme conditions***

Nanometer sized particles, droplets or crystals, form both in the environment and in large scale industrial processes. Accurate predictions of the phase transition rates, and the phase or structure of the particles, are critical for developing reliable models of industrial processes, climate, and atmospheric chemistry. Particles with radii < 10 nm are also of fundamental because they lie in the critical transition zone between large molecular clusters and bulk materials. For small enough particles, internal droplet pressure can easily reach ~30 MPa. This talk will summarize our work following freezing of highly super-cooled water using techniques that include small angle x-ray scattering (SAXS), wide angle X-ray scattering (WAXS), infrared spectroscopy, and pressure measurements. For water, the small droplet size and the rapid cooling rate means that liquid water only begins to freeze below ~225 K – a temperature that is well below the homogeneous freezing limit for bulk water or even micron size water droplets. These experiments show the expected decrease in freezing temperature with decreasing droplet size, or alternatively, with increasing droplet internal pressure. The final phase of the ice is also highly cubic ice I rather than the more stable hexagonal ice I.

**Sotiris Xantheas,** Pacific Northwest National Laboratory

***Liquid water is markedly different than liquid H2X (X = S, Se, Te)***

Among liquid water's many anomalous properties, the high melting, boiling and critical points compared to the ones of the rest of chalcogen hydrides (H2S, H2Se, H2Te) 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 H2X (X = S, Se, Te). Angular distribution functions confirm the well-known result that each H2O 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 H2S to H2Te but are starkly different from those of water. Our results demonstrate that water forms an exceptionally different liquid from H2S, H2Se, and H2Te, 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.

**Limei Xu,** Peking University

***Ice Crystallization and premelting in low dimensions: an atomic-scale view***

The structure and dynamics of water at the atomic scale play crucial roles in atmospheric, materials, and biological processes. However, the mechanisms of crystallization and melting in interfacial and low-dimensional systems remain poorly understood, and the applicability of classical theories in these regimes remains an open question. We combine cryogenic atomic force microscopy, molecular dynamics simulations, and machine learning methods to investigate ice interfacial structures and phase transitions at atomic resolution. We find that crystallization in two-dimensional ice exhibits strongly non-classical behavior, where three-dimensional water molecules at the interface promote ordering within the 2D ice layer. Furthermore, ice surfaces contain multiple locally ordered structures with different symmetries, and premelting preferentially initiates at the boundaries between these distinct domains. Across the temperature range from low temperatures to near melting, we identify a previously unknown amorphous intermediate state between the crystalline phase and the quasi-liquid layer. This state exhibits a disordered hydrogen-bond network with solid-like dynamics, revealing a continuous structural evolution from crystal to liquid-like behavior. This work provides a new microscopic perspective on interfacial phase transitions of water.