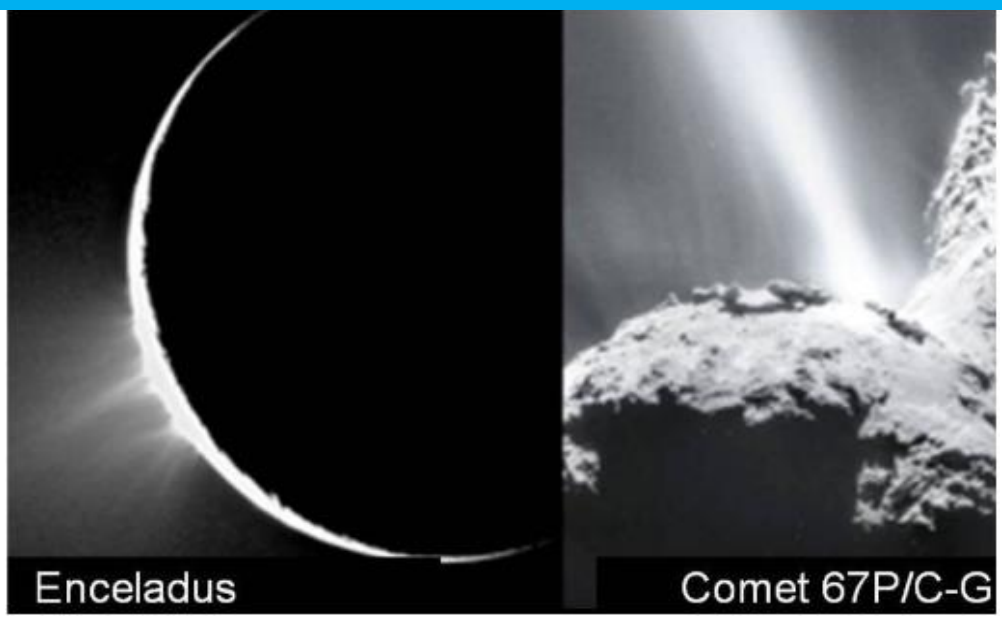
Newsletter #1

CMWS
Centre for Molecular Water Science



Plumes of water and methane issuing from fissures in overlying ice. Left: Cassini image of the South pole of Enceladus; Rosetta image of jet of water and organics in comet 67P/C-G. Copyright: Journal of Cosmology, Vol. 30, No. 3, pp. 30030 - 30034

Dear CMWS colleagues,

It is with great pleasure to present to you the first CMWS newsletter. We plan to make this a regular activity with two to three newsletters a year to keep everyone informed also "between the CMWS Water Days". This newsletter will report on recent research findings of CMWS colleagues as well as past and planned CMWS activities and other molecular-water related events. We also provide a "people" section to introduce colleagues to the network from a maybe slightly different perspective and are happy to announce open positions if you are seeking for suitable candidates. In future editions, we will also present the so far available CMWS instrumental infrastructure to you.

There are exciting plans for the next semester and the near future: There will be another targeted, challenge-driven call for PETRA III beamtime with a focus on molecular-water research, as also outlined in this newsletter. Furthermore, as many of you know, we are currently preparing a proposal to apply for funding within the Helmholtz association for the building and infrastructure of a CMWS central hub and to generally strengthen the CMWS hub structure.

In addition, we are currently in the process of preparing a CMWS Graduate Workshop, which will take place from November, 15th-17th 2023. It will address the highly interdisciplinary character of the CMWS with tailored lectures on experimental and theoretical approaches as well as strengthen the network of the younger researchers.

We would also like to recommend our biweekly CMWS seminar, which offers exciting insights into research topics and regularly brings us together for interesting discussions. It is held online and takes place every second Thursday. Note that we changed the time to 2 p.m., which hopefully makes it better suited for most of you.

Finally, we would like to encourage all CMWS members to seek and make use of the contacts with other members that the CMWS network offers – for the mutual exchange of expertise, for joint initiatives and projects, or to simply chat among scientists.

Enjoy reading the newsletter. We look forward to any constructive feedback on this format that you may have.

With best regards,

your CMWS Team

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Last update: 12.09.2023

INSIDE CMWS

Scientists gather at the CMWS Water Days 2023

From 21-24th of February 2023, the CMWS WATER DAYS 2023 took place in Hamburg. Researchers from 20 countries met to discuss the key challenges in molecular water research and the status and future of the CMWS.

Several plenary talks addressing recent results from theory and experiment inspired discussions. Special workshops took place on funding opportunities as well as on establishing the CMWS in a more European setting.

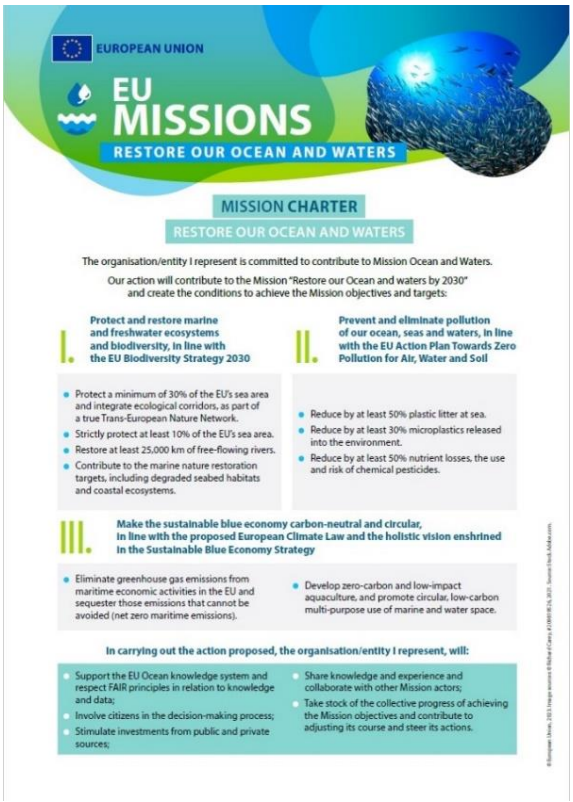
One highlight was a public evening lecture delivered by Prof. Katrin Amann-Winkel, where she introduced us and the interested public to "Ice Under Pressure – Exploring the Crazy Properties of Water".

As a part of the CMWS WATER DAYS 2023, the 20th annual DESY Research Course for students, young research fellows, and interested scientists was focused on "Water in Climate-, Astro and Geo Sciences", which is an essential part of the CMWS research agenda. Several lectures gave an impressive overview from the relevance of molecular water in space as well as in the interior of planets, in the oceans, and high pressure and under the almost vacuum-like conditions in space. The diverse applications triggered rich discussions among the participants.

CMWS Endorses the Ocean and Waters Mission Charter

CMWS and DESY as its host institution endorsed the EU Mission Charter "Restore our ocean and waters". With this endorsement, the CMWS is part of a larger network to contribute to one or more of the following Mission Ocean and Waters objectives:

- Protect and restore marine and freshwater ecosystems and biodiversity, in line with the EU Biodiversity Strategy 2030
- Prevent and eliminate pollution of our ocean, seas and waters, in line with the EU Action Plan Towards Zero Pollution for Air, Water and Soil
- Make the sustainable blue economy carbon-neutral and circular, in line with the proposed European Climate Law and the holistic vision enshrined in the Sustainable Blue Economy Strategy



CMWS Logo and acknowledging the CMWS

To increase the visibility of the CMWS at the national and international level, we encourage you to add CMWS to the acknowledgement of your publications.

"We acknowledge the scientific exchange and support of the Centre for Molecular Water Science (CMWS)."

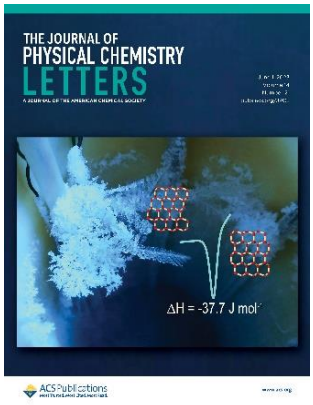
For all publications of early science and science projects, it is mandatory to include CMWS in the acknowledgement: "This research was supported by the Centre for Molecular Water Science (CMWS) as an Early Science Project".

CMWS logo for download:

About CMWS (cmws-hamburg.de)

HIGHLIGHTS & RESEARCH

Enthalpy Change from Pure Cubic Ice I_c to Hexagonal Ice I_h



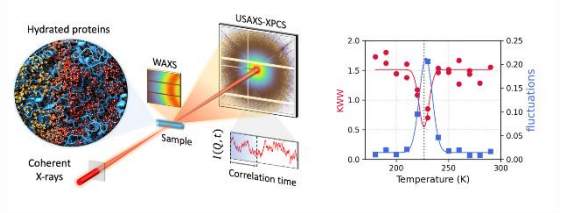
The preparation of pure cubic ice without hexagonal stacking faults has been realized only recently by del Rosso et al. (Nat. Mater. 2020, 19, 663−668) and Komatsu et al. (Nat. Commun. 2020, 11, 464). With our present calorimetric study on the transition from pure cubic ice to hexagonal ice, we are able to clarify the value of the enthalpy change ΔHc→h to be −37.7 ± 2.3 J mol–1. The transition temperature is identified as 226 K, much higher than in previous work on ice Isd. This is due to a catalytic effect of hexagonal faults on the transition, but even more importantly due to a relaxation exotherm that was not properly identified in the past (Tonauer, C. M., Yamashita, K., Rosso, L. del, Celli, M., & Loerting, T. (2023). Enthalpy Change from Pure Cubic Ice Ic to Hexagonal Ice Ih. The Journal of Physical Chemistry Letters, 14(21), 5055–5060). https://doi.org/10.1021/acs.jpclett.3c00408

Nucleation and growth of crystalline ices from amorphous sources

Nucleation of ice is a highly relevant process in many fields, such as biology (e.g., for the survival of plants and animals at subzero temperatures), cloud physics or in industry (e.g., for the prevention of icing on aeroplanes or the production of technical snow). Nucleation is the initializing mechanism of crystallization, followed by growth of crystals. Despite its importance, so far there are only a handful of studies in which crystal nucleation and growth from amorphous ices are investigated as two separate processes. The present review includes mostly experimental and some computational work devoted to nucleation in amorphous ices, namely vapour-deposited amorphous solid water (ASW), hyperquenched-glassy water (HGW), low-density amorphous ice (LDA), high-density amorphous ice (HDA) and very high-density amorphous ice (VHDA), covering the pressures up to 6 GPa and temperatures up to 270 K. The role of sample preparation and strategies for disentangling nucleation from the growth process (e.g., "intentional preseeding") for tackling open questions are discussed (Tonauer, C. M., Fidler, L.-R., Giebelmann, J., Yamashita, K., & Loerting, T. (2023). Nucleation and growth of crystalline ices from amorphous ices. The Journal of Chemical Physics, 158(14), 141001). https://doi.org/10.1063/5.0143343

Coherent X-ray Scattering Reveals Nanoscale Fluctuations in Hydrated Proteins

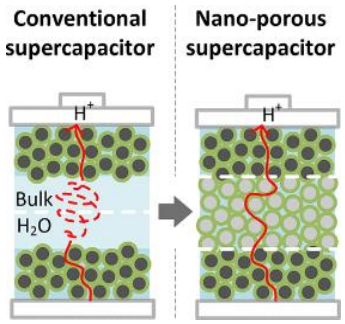
Hydrated proteins undergo a transition in the deeply supercooled regime, which is attributed to rapid changes in hydration water and protein structural dynamics. Here, we investigate the



nanoscale stress-relaxation in hydrated lysozyme proteins stimulated and probed by X-ray Photon Correlation Spectroscopy (XPCS). This approach allows us to access the nanoscale dynamics in the deeply supercooled regime (T = 180 K), which is typically not accessible through equilibrium methods. The observed stimulated dynamic response is attributed to collective stress-relaxation as the system transitions from a jammed granular state to an elastically driven regime. The relaxation time constants exhibit Arrhenius temperature dependence upon cooling with a minimum in the Kohlrausch-Williams-Watts exponent at T = 227 K. The observed minimum is attributed to an increase in dynamical heterogeneity, which coincides with enhanced fluctuations observed in the two-time correlation functions and a maximum in the dynamic susceptibility quantified by the normalized variance. The amplification of fluctuations is consistent with previous studies of hydrated proteins, which indicate the key role of density and enthalpy fluctuations in hydration water. Our study provides new insights into X-ray stimulated stress-relaxation and the underlying mechanisms behind spatiotemporal fluctuations in biological granular materials (Bin, M., Reiser, M., Filianina, M., Berkowicz, S., Das, S., Timmermann, S., Roseker, W., Bauer, R., Öström, J., Karina, A., Amann-Winkel, K., Ladd-Parada, M., Westermeier, F., Sprung, M., Möller, J., Lehmkühler, F., Gutt, C., & Perakis, F. (2023). Coherent X-ray Scattering Reveals Nanoscale Fluctuations in Hydrated Proteins. The Journal of Physical Chemistry B, 127(21), 4922–4930).

https://doi.org/10.1021/acs.jpcb.3c02492

Confinement-Controlled Water Leads to Unusually High Electrochemical Capacitance

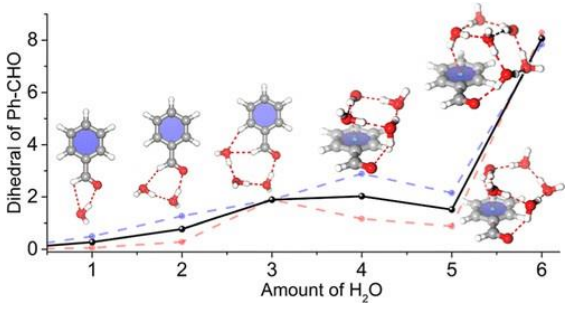


The remarkable electrochemical properties of confined water in nanopores are studied, relevant for the development of a nanofluidic 'water-only' battery. By exploiting the unique behavior of water under strong confinement, we achieve unusually high electrolytic properties and energy density. Our findings challenge the current limitations of metal-ion batteries and pave the way for low-cost and environmentally safe energy storage solutions in the renewable energy sector. The optimal pore size for maximizing performance is determined to be 3 nm, highlighting the significance of nanoconfined water dynamics in energy storage applications. This research opens up new avenues for sustainable and efficient electrochemical systems that harness the intrinsic properties of water (Melnik, S., Ryzhov, A., Kiselev, A., Radenovic, A., Weil, T., Stevenson, K. J., & Artemov, V. G. (2023). Confinement-Controlled Water Engenders Unusually High Electrochemical Capacitance. The Journal of Physical Chemistry Letters, 14(29), 6572–6576.

https://doi.org/10.1021/acs.jpclett.3c01498

Intriguing change in micro-solvation pattern – the case of benzaldehyde-water complexes

The investigation on the preferred structural arrangements and intermolecular interactions of gas-phase solute−water clusters can give insights into the intermolecular potentials that govern the structure and dynamics of aqueous solutions. Here, we report the investigation of hydrated coordination networks of benzaldehyde-$(water)_n$ (n = 1−6) complexes under the cold conditions of a pulsed supersonic expansion using broadband rotational spectroscopy. This method provides precise experimental structures, which can for example be used to benchmark theoretical models. Benzaldehyde, C_6H_5CHO, is the simplest aromatic aldehyde that involves both hydrophilic (the aldehyde group, CHO) and hydrophobic (the phenyl ring) functional groups, and which can thus mimic molecules of biological relevance.



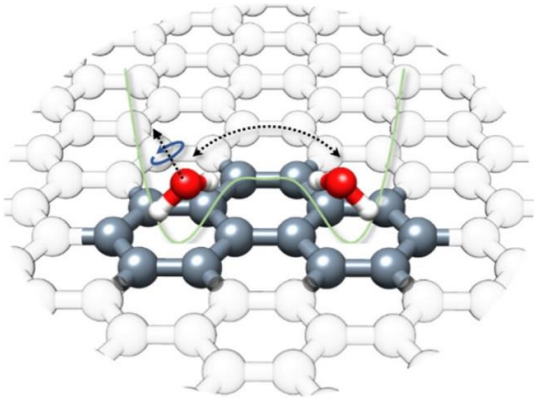
Interestingly, we observe a dramatic change in water-molecule arrangement with increasing number of water molecules: For the n=1-3 complexes, the water molecules are located in-plane with respect to the benzaldehyde molecule and connected around the hydrophilic aldehyde group through a strong CO···HO hydrogen bond and weak CH···OH hydrogen bond(s).

For the larger clusters (n=4-6), the spectra are consistent with the structures in which the water molecules are coordinated on the surface of PhCHO in a sandwich-like arrangement, instead of in the plane as for the complexes with less water molecules. The presence of benzaldehyde does not strongly interfere with the cyclic water tetramer and pentamer, which retain the same structure as in the pure water cluster. For the water hexamer, we observe exclusively the book isomer instead of its cage or prism isomers as complex partner for benzaldehyde. Interestingly, also the solute, benzaldehyde, starts to deviate from the planar structure upon sequential addition of water molecules. The PhCHO−$(H_2O)_{1-6}$ clusters may serve as an interesting model system in understanding the solute−water interactions of biologically relevant molecules in an aqueous environment (Li, W., Pérez, C., Steber, A. L., Schnell, M., Lv, D., Wang, G., Zeng, X., & Zhou, M. (2023). Evolution of Solute–Water Interactions in the Benzaldehyde-(H2O)1–6 Clusters by Rotational Spectroscopy. Journal of the American Chemical Society, 145(7), 4119–4128). https://doi.org/10.1021/jacs.2c11732

Quantum Tunneling Facilitates Water Motion across the Surface of Phenanthrene

Understanding the diffusion of water molecules on carbon surfaces, like graphene, is a fundamental step towards comprehending various complex physical and chemical phenomena that occur in our everyday lives and in scientific and technological processes, such as corrosion, catalysis, electrochemistry, ice nucleation, and separation technologies, to name a few. However, studying the interaction between a single water molecule and a carbon surface has proven to be a challenging task due to the high propensity of water molecules to form hydrogen bonds, which results in rapid formation of water clusters, and the high mobility of water's protons. These factors make it difficult, for example, for imaging techniques to capture the water's behavior when interacting with such surfaces.

We exploited the outstanding high resolution of broadband rotational spectroscopy to disentangle in detail the complex internal dynamics of a single water molecule when interacting with the planar carbon surface of phenanthrene, which served as a small-scale carbon-surface like model. Our findings revealed that the diffusion of a single water molecule on carbon surfaces occurs via quantum tunnelling of the water molecule between one aromatic ring of phenanthrene and the equivalent one.



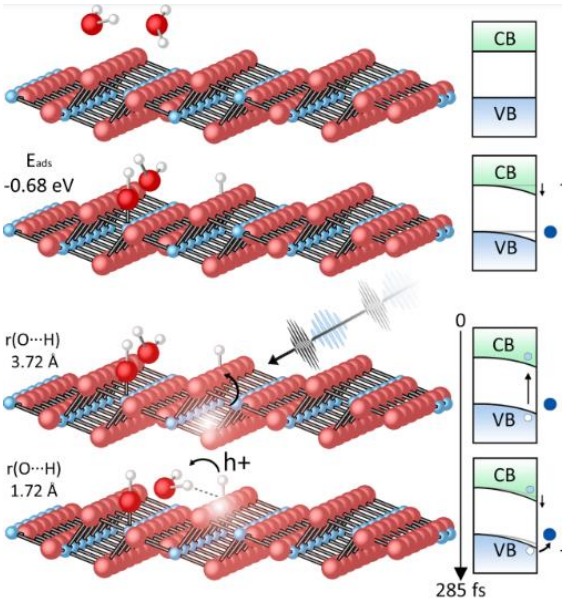
The water's migration pathway was disentangled in detail by investigating the effect of isotopic substitution on the line splitting in the rotational spectra of the $H_2{}^{16}O$, $H_2{}^{18}O$, D_2O and HDO isotopologues of the monohydrated cluster of phenanthrene. This study shows that the water molecule diffuses via a concerted tunnelling motion which involves the simultaneous internal rotation of the water molecule along its internal symmetry axis and its translation between the two peripheral rings of phenanthrene. These findings provide a valuable small-scale model to help disentangle water's diffusion on more complex carbon surfaces, such as large polycyclic aromatic hydrocarbons or graphene (Loru, D., Steber, A. L., Pérez, C., Obenchain, D.A, Temelso, B., López, J. C., Schnell, M. (2023). Quantum Tunneling Facilitates Water Motion across the Surface of Phenanthrene. Journal of the American Chemical Society, 145, 31, 17201–17210). https://doi.org/10.1021/jacs.3c04281

Ultrafast light-induced dynamics in the microsolvated biomolecular indole chromophore with water

A sophisticated experiment provides new insights into the ultrafast reaction of (biomolecules when they are hit by energetic ultravioletmicro) solvated light in their natural environment. The light-induced ultrafast processes taking place in a prototypical molecule-water were studied. This aggregate served as model system for the interactions between proteins and surrounding solvent molecules, usually water. The experiment is an important step on the way to record a "molecular movie" of such chemical reactions (Onvlee, J., Trippel, S., & Küpper, J. (2022). Ultrafast light-induced dynamics in the microsolvated biomolecular indole chromophore with water. Nature Communications, 13(1), Article 1). https://doi.org/10.1038/s41467-022-33901-w

Photoinduced Dynamics at the Water/TiO_2(101) Interface

We present a femtosecond time-resolved optical pump-soft x-ray probe photoemission study in which we follow the dynamics of charge transfer at the interface of water and anatase TiO_2(101). By combining our observation of transient oxygen O 1s core level peak shifts at submonolayer water coverages with Ehrenfest molecular dynamics simulations, we find that ultrafast interfacial hole transfer from TiO_2 to molecularly adsorbed water is completed within the 285 fs time resolution of the experiment. This is facilitated by the formation of a new hydrogen bond between an O_{2c} site at the surface and a physisorbed water molecule. The calculations fully corroborate our experimental observations and further suggest that this process is preceded by the efficient trapping of the hole at the surface of TiO_2 by hydroxyl species (-OH), that form following the dissociative adsorption of water. At a water coverage exceeding a monolayer, interfacial charge transfer is suppressed. Our findings are directly applicable to a wide range of photocatalytic



systems in which water plays a critical role (Wagstaffe, M., Dominguez-Castro, A., Wenthaus, L., Palutke, S., Kutnyakhov, D., Heber, M., Pressacco, F., Dziarzhytski, S., Gleißner, H., Gupta, V. K., Redlin, H., Dominguez, A., Frauenheim, T., Rubio, A., Stierle, A., & Noei, H. (2023). Photoinduced Dynamics at the Water / TiO_2 (101) Interface. PHYSICAL REVIEW LETTERS, 130(10), 108001). https://doi.org/10.1103/PhysRevLett.130.108001

ANNOUNCEMENTS

Winter Semester 2023

We are happy to announce a brand-new series of CMWS seminars for the winter term as well as exciting workshops.

Seminar Series

We are delighted to announce the upcoming seminar series for the winter semester of 2023, with a slight change in the schedule. The biweekly seminars will now be held on Thursdays at **14:00 via Zoom**. We are currently in the process of finalizing the program.

NOW at 14:00!

- 19.10.23 - Mariana Rossi (Center for Free-Electron Laser Science (CFEL) & Max Planck Institute for the Structure and Dynamics of Matter)
- 02.11.23 - Ellen Adams (TU Dresden, HZDR)
- 30.11.23 Hans-Jürgen Butt (MPI für Polymerforschung)

Further seminars are taking place on 16.11.23, 30.11.23, 14.12.23, and 11.01.24.

SAVE THE DATE!

Match-Making for the next Targeted Challenge-Driven Call at PETRA III

DESY Photon Science offers to all PETRA III users the possibility to apply for Targeted Challenge-Driven (TCD) proposals at PETRA III on "Molecular Water Science". The call for TCD proposals will be opened mid of October 2023. The deadline for proposal submission will be March 1st, 2024. This call is intended for collaborations of at least three research groups who work on challenging topics in molecular water science. To enable comprehensive and high-impact studies, DESY offers access to several beamlines at PETRA III during a 2-year TDC project phase. Prerequisites for successful proposals are: a clear description of the project, an elaborated project plan, well-formulated goals, and clear evidence for a strong cooperation of the partners within the project.

Interested groups have the option to learn about the TCD-call for "Molecular Water Science" and find partners for projects on this match-making workshop:

PETRA III: Targeted Challenge Driven Proposals "Molecular Water Science"

When: 5th of October 2023
From 13:30 - 18:30
Where: CSSB Auditorium (DESY - Notkestraße 85, 22607 Hamburg) followed by dinner

https://indico.desy.de/event/40308/

Please register if you want to participate!

CMWS Graduate Workshop -Coming soon!

With three successful rounds of the Science Program, the Centre for Molecular Water Science is organizing the 1st CMWS Graduate Workshop, taking place on the DESY campus in Hamburg from November 15th to 17th, 2023.

The workshop aims to bring together young scientists from across the different research pillars. Everyone affiliated with the CMWS and the Science Program, or simply interested in molecular water science, is welcome to join and share their latest research results. Particularly those working on the (Early) Science Program are strongly encouraged to participate and share recent highlights of their

projects. The event will entail poster sessions where all participants can present their work, talks by advanced scientists covering a variety of experimental and theoretical techniques,

SAVE THE DATE!

CMWS Graduate Workshop
When: 15th - 17th of November 17, 2023
Where: DESY

and will end with the Hamburg Photon Science Colloquium.

We will follow up with more details about the registration and program soon but please save the date!

Research activities at Geolab Reiche Zeche

ZeWaF welcomes students and postdocs to attend a workshop and networking opportunity Friday, September 22nd, 2023, featuring selected presentations and a tour of the Reiche Zeche Geolab facility.
Reiche Zeche is a silver mining facility dating back to 1384, at the heart of TU Bergakademie Freiberg. Although mining ceased in 1969, it now houses a vast array of research infrastructure. Presentations focus on various aspects of water in mines, with specific emphasis on the current activities at the Geolab Reiche Zeche. Topics will range from bio-leaching of metals and shock wave laboratory work, to using detection robots underground and more.

When: September 22, 2023
Location: Reiche Zeche, Freiberg
Hosted by: TU Bergakademie Freiberg, ZeWaF

For additional information and registration please contact the ZeWaF team by email. (zewaf@tu-freiberg.de).

CAREER & OPEN POSITIONS

Investigating solvent effects in the dynamics of biologically relevant model systems

The Controlled Molecule Imaging group at CFEL, DESY has an open doctoral-student position in a research project studying the influence of microsolvation on the ultrafast elementary steps of biomolecular chemical dynamics. The research builds upon the forefront of solvated-molecule preparation and imaging techniques available in our group and the ultrafast-laser experience of our collaborators. This project is part of the HELIOS graduate school and in close collaboration with Francesca Calegari in Hamburg and partners in Lund (Per Johnsson and Mathieu Gisselbrecht).

Novel approach to sample preparation for high-resolution cryo-EM

The Controlled Molecule Imaging group at CFEL, DESY has an open postdoc position in a research project aiming at a new, disruptive sample-delivery technique for cryogenic-electron-microscopy applications. You will for on preparing "wet" solvated biomolecules in the gas-phase for shock freezing and soft-landing approaches. The work is in close collaboration with the Marlovits group at CSSB and an industrial partner.

Further information about both of these positions is available here https://www.controlled-molecule-imaging.org/careers

PEOPLE IN THE COMMUNITY

We have had the privilege of interviewing Nønne Prisle from Oulu University, Richard J. Saykally from the University of California, and Katinka Horn from DESY & ETH Zürich. Meet them in the interviews below and get some ideas about their views on science, molecular water and life.

Nønne Prisle

How did you get into molecular-water-related research?

Nønne: After my B.Sc. thesis in theoretical physics on seismic waves, I became interested in the science of climate change, global warming, and atmospheric chemistry. For my M.Sc., a mentor nudged me towards aerosol and cloud research, which was an emerging topic at the time. The theory of cloud formation is deceptively simple, but as soon as you look a bit closer, it is both complex and fascinating. When water condenses on the surface of a nano-particle, it initiates both thermodynamic and chemical processes and displays properties of both quantum and bulk systems. There are still many things we simply don't know about cloud droplet formation and have no way to reliably measure or calculate. My work has developed methods to measure and calculate some of these unknowns and contributed to solving a few questions, but there is so much more still to discover.

Please tell us about your latest research project.

Nønne: In two previous large projects, my team and I have applied synchrotron X-ray spectroscopy and imaging to characterize samples resembling atmospheric aerosols and cloud droplets to varying degrees. Here, we have learned a lot about the challenges related to experimental conditions and requirements. Our latest project focuses on overcoming challenges in complex data analysis and use of the data from these experiments in atmospheric and climate models. One strategy is to apply new machine learning methods to achieve this. We hope to be able to take even better advantage of the new possibilities at advanced light sources.

Which open question or challenges in molecular-water related research would you like to see answered in the near future?

Nønne: I am very interested in how different forms of nano-scale confinement affects the processes in cloud droplets, and how we can develop our models to represent such effects.

What was the most important advice someone gave you?

Nønne: I have been very fortunate to get a lot of good advice from many different people over the years! It is very difficult to pick one piece as the most important. But, if I try, it must be that, when faced with difficult decisions, we often know very well what we what to do, the difficult part is not to decide, but to justify our decision, to ourselves, and anyone else who has a stake in it. Once, when I asked a mentor for advice to make such a difficult decision, and when I had listed all the pros and cons, he just said to "make the decision with the heart, because even if it turns out to be the wrong one, you will rarely regret it". To this day, it still holds.

When do you have your best ideas?

Nønne: Just before falling asleep, when the brain is still somewhat awake, but with less executive supervision. I always keep a notebook on the bedside table. This is, however, also when I get my "worst" ideas. I still keep those ideas, and plan to use them for a comic book of sorts, which I will write when I retire.

What does make you laugh?

Nønne: My partner. He is a fellow scientist and a seemingly infinite source of nerdy and clever jokes with a subversive streak. Sometimes, he isn't even trying to be funny but still succeeds! I also have a soft spot for cat videos, one of the greatest things of social media.

How do you balance your professional and personal life?

Nønne: To be honest, there are times when this is not straight-forward. For me, science has been a way of life for a very long time. I met my partner and many dear friends in the lab, on campaigns, at conferences, or as co-authors of papers. I enjoy discussing unsolved questions and new ideas in

science. Nowadays, there are also many administrative tasks that simply need to be taken care of so that our research can run smoothly. A simple and effective trick I learned while working from home during Covid is to clear my desk at the end of the day, close all files and tabs, put all papers in folders, and the folders into a cabinet, and make a task list for next morning. That takes most off my mind. I also prioritize doing some sports on most days, if the weather is not too bad. After more than a decade in Finland, I have learned that there is basically no such thing as too bad weather for sports. When I really need a break, I start to tackle a practical task that is sufficiently demanding that it will take all my efforts for some hours or days, often in the garden or around the house. I can also always rely on my family and childhood friends to remind me of life outside the office.

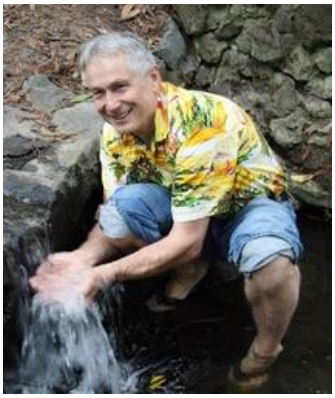
Where can you be found when you are not doing water-related research?

Nønne: Outside, under the sky, either running, or working in my garden, tending to my fruit trees and berry bushes. Although this may sound very peaceful, it can actually be quite labor intense. There is a surprising amount of chain-sawing and axing involved in being a tree-hugger. I also really enjoy growing trees all the way from seeds. We are still learning new ways to use the bounties of the trees and bushes, so far we have mastered a range of pies, cakes, jams, and other preserves.

And which advice can you give to young researchers in the field?

Nønne: There are many things I wish I had known a long time ago! It is important to develop your own unique way and to continue to learn new things, by discussing and collaborating with people somewhat outside of what you are currently doing. And while excellent scientific skills are naturally the foundation for building your scientific career, perseverance, communication, and collaboration are all key to going far.

Rich Saykally



How did you get into molecular-water-related research?

Rich: We developed terahertz laser vibration-rotation-tunneling spectroscopy of weakly bound clusters back in 1990, with the goal of extracting highly detailed potential energy models for them; we then progressed into studying the water dimer. Comparisons of spectra predicted with the prevailing theoretical water models didn't agree with our measurements. We progressed to the study of water trimers, tetramers, pentamers, hexamers, octamers and the disagreement with theory became even worse. We then worked with theoreticians to use our water cluster data to develop a "universal first principles' water model", which would work for both clusters and bulk water properties. This has now been largely realized, thanks to the work of many students, postdocs, and theoretical collaborators. The point has now been reached wherein one can ask essentially any question about water, and these new water models can provide a believable answer. Meanwhile, practical issues involving water have moved to the forefront of science and engineering because of the fundamental importance of water to our world.

Please tell us about your latest research project.

Rich: Trying to understand all the details of carbon dioxide adsorption and subsequent chemistry by our oceans

Which open question or challenges in molecular-water related research would you like to see answered in the near future?

Rich: Same as above

What was the most important advice someone gave you?

Rich: "Life is short!! Have fun!!" "Science is fun!!"

When do you have your best ideas?

Rich: While reading the literature. I like to read a lot.

What does make you laugh?

Rich: Stupid politicians!

How do you balance your professional and personal life?

Rich: I make sure to incorporate some intense physical exercise (bike riding, walking, weight exercise) into each day, spend time with my wife and daughters, play some music, meet up with friends…

Where can you be found when you are not doing water-related research?

Rich: In a good pub, playing music and arguing with friends!

And which advice can you give to young researchers in the field?

Rich: Have fun!! Search for questions that excite you! Remember the motto of the UK Royal Society: "Nullius in verba", taken to mean "take nobody's word for it"; verify all statements by appealing to facts determined from experiment.

Katinka Horn

Please tell us about your latest research project.

Katinka: The first two years of my Joint PhD I spent in Zürich, doing research in the Aerosols and Nanoscience group led by Ruth Signorell at ETHZ. We investigate electron scattering in neutral nanometer-sized water clusters by means of photoelectron spectroscopy. We use the experimental data to develop a detailed electron scattering model for low energy electrons in water (< 50 eV). We look at an energy regime where different scattering channels (inelastic/elastic ones) turn on and off. Now I transfer to the CFEL-ATTO group led by Francesca Calegari at DESY, where one aim is to do time-resolved measurements of the electron scattering. It is really fun, you should come and visit!

Which open question or challenges in molecular-water related research would you like to see answered in the near future?

Katinka: What would really help me in my research is to know the dielectric function of water in response to quasi-free electrons in the energy range from 10 – 50 eV.

What was the most important advice someone gave you?

Katinka: You do you.

What does make you laugh?

Katinka: Situational comedy.

And which advice can you give to young researchers in the field?

Katinka: Be water, my friend.

CONFERENCES & WORKSHOPS OVERVIEW

2023

The 7th edition of the SMARTER

September 17 – 21, 2023, KU Leuven, Belgium

The 7th edition of the SMARTER

Research activities at Geolab Reiche Zeche

September 22, 2023. TU Bergakademie Freiberg, ZeWaF

For additional information send an Email to zewaf@tu-freiberg.de

Match-Making for the next Targeted Challenge-Driven Call at PETRA III

October 5, 2023, DESY, Hamburg. Germany

https://indico.desy.de/event/40308/

CMWS Graduate Workshop

November 15- 17, 2023. DESY, Hamburg. Germany

https://www.cmws-hamburg.de/news_amp_events/news/2023/save_the_date/

2024

18th International Conference on the Properties of Water and Steam

June 23-28, 2024. Boulder, Colorado, USA

18th International Conference on the Properties of Water and Steam (iapws.org)

Water and Aqueous Solutions (GRS)

July 20 - 21, 2024. Holderness, NH, United States

2024 Water and Aqueous Solutions (Gordon Research Seminar)

-SAVE THE DATE-

Water and Aqueous Solutions (GRS)

July 21 - 26, 2024. Holderness, NH, United States

2024 Water and Aqueous Solutions Conference (Gordon Research Seminar)

Liquid Matter Conference 2024

September 22 – 27, 2024. Mainz

12th Liquid Matter Conference

EMLG–JMLG Annual Meeting 2024

September 8 – 13, September 2024, Trieste, Italy

Structure and Dynamics of Hydrogen- bonded Liquid Systems