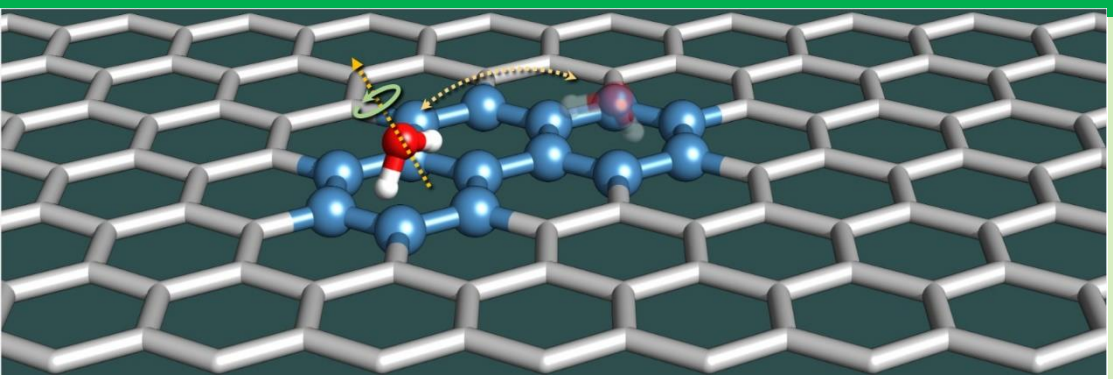
Newsletter #2



The dynamics of an individual water molecule on the planar surface of the polycyclic aromatic hydrocarbon phenanthrene was explored using high-resolution broadband rotational spectroscopy. The water molecule shows a concerted tunneling motion involving its internal rotation and translation as it shuttles between the two equivalent peripheral rings of phenanthrene. (Loru. 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

Dear CMWS colleagues,

It is with great pleasure to share with you the second CMWS newsletter, where we would also like to take the opportunity to look back at some of the 2023 activities within the CMWS.

We saw the start of several new joint projects within the CMWS Science program, we met many of you in person at the CMWS Water Days 2023, virtually at the seminars, and we had intense exchange especially among the younger researchers at the recent CMWS graduate workshop that took place just a few weeks ago. Coordinated by Eric Breynaert and his team, the CMWS IDNET proposal was handed in to the EU call for doctoral networks. Fingers crossed for a successful application, and a great thanks to all who contributed. We formulated and discussed a joint CMWS declaration, and 42 partners agreed to sign this declaration and thus become founding members. We plan a corresponding festive event in summer 2024 and will keep you informed.

In this issue of the newsletter, we will report the latest research findings of CMWS colleagues as well about past and planned CMWS activities and other molecular-water related events. We are especially happy to announce the next CMWS Water Days, this time taking place from 26.02.-28.02.2024, with registration starting in January 2024. We plan with a dedicated session of contributed talks, where everyone interested can submit an abstract, also with the aim to identify new collaborations. In another session, we plan to introduce some of the already existing CMWS hubs and infrastructure offers to all CMWS members.

In the “people” section we interviewed Fivos Perakis from Stockholm University, Yongjae Lee from Yonsei University in Seoul, and Gavriel Arbiv from KU Leuven. As we approach the holiday season, we extend warm wishes to all CMWS members for a Merry Christmas and a Happy New Year filled with fresh ideas and exciting results.

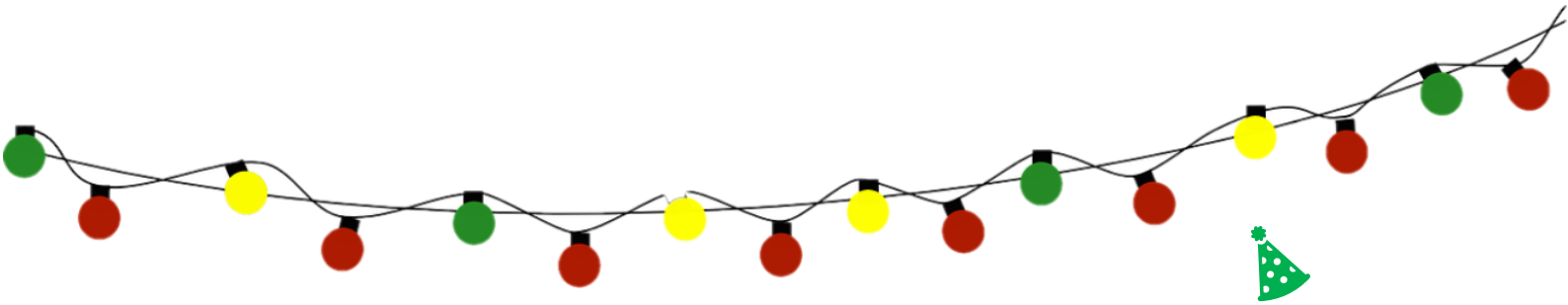
With best regards,
The CMWS team

Inside CMWS

Research

SAVE THE DATE

People – Meet our community



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CMWS logo for download About CMWS (cmws-hamburg.de)

Last update: 22.12.2023

Students gather at the CMWS graduate days 2023

The 1st CMWS Graduate Workshop took place from November 15th to 17th at the DESY Campus. About 50 early career researchers got together with well-recognized experts from different fields of molecular water science and shared ideas and the latest highlights of their work. The workshop featured poster presentations as well as invited talks covering topics from water filtration to real-time molecular dynamics. Participants also had the opportunity to attend a tour of the European XFEL, concluding the night with bowling as a social activity. The workshop ended with the Hamburg Photon Science Colloquium given by Jaydeep Basu from IISc Bangalore talking about his research and application of quantum dots.

Call for targeted challenge-driven (TCD) proposals at PETRA III on "molecular water science" & FLASH

The match-making workshop related to the upcoming second call for targeted challenge-driven (TCD) proposals at PETRA III & FLASH on "molecular water science" took place on October 5th, 2023 at DESY Campus.

During this workshop, interested user groups were briefed about this call and encouraged to find partners for collaborative projects for match-making. Participants registered by providing a summary of their interest in "Molecular Water Science," which was shared among all attendees.

For further information about this event, please visit: PETRA III & FLASH: Targeted Challenge Driven Proposals "Molecular Water Science" (October 5, 2023): Overview · DESY-Konferenzverwaltung (Indico)

The related call for TCD proposals will be opened in January 2024. The deadline for proposal submission is set for March 1st, 2024

Submit your proposal here:
DESY Photon Science - DOOR

New Emmy Noether group for Florian Trinter

Florian Trinter has been connected with the CMWS since the very early days and contributed to the White Paper (Pillars 2 and 4). His (future) research is closely associated with Pillar 4: Real-Time Chemical Dynamics. He is looking forward to actively contributing to the scientific challenges in the characterization of the energetics and dynamics of the transient radicals produced by water radiolysis with his new independent Emmy Noether group awarded by the Deutsche Forschungs-gemeinschaft. His main focus will be on the time-

resolved interrogation of photogenerated transient electrons, protons, and radicals, including their formation mechanisms, propagation, structure, and reaction dynamics in solvated complexes in bulk aqueous solution and at the solution-vacuum interface. The envisioned vis-UV laser pump / soft X-ray probe photoelectron-spectroscopy studies will be enabled by synchronizing a dedicated tunable picosecond laser to the PETRA III master clock. Aqueous-phase targets are delivered either by cylindrical microjets or flatjets. Florian Trinter has already contributed to numerous CMWS-related publications, not only on liquid-jet photoelectron spectroscopy, but also covering PETRA III-based electron-ion coincidence spectroscopy of biomolecules in aqueous environments and X-ray absorption spectroscopy of oxonium ions as well as EuXFEL-based multi-ion coincidence spectroscopy of molecular water.

The complete press release can be found here https://www.fhi.mpg.de/1373817/2023-10-

HIGHLIGHTS & RESEARCH

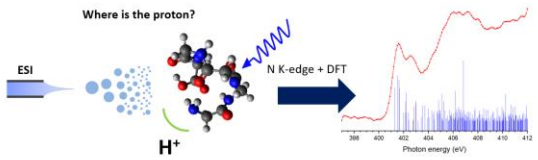
Graphite resistive heated diamond anvil cell for simultaneous high-pressure and high-temperature diffraction experiments

High-pressure and high temperature experiments using a resistively heated diamond anvil cell have the advantage of heating samples homogeneously with precise temperature control. Here, we present the design and performance of a graphite resistive heated diamond anvil cell (GRHDAC) setup for powder and single-crystal x-ray diffraction experiments developed at the Extreme Conditions Beamline (P02.2) at PETRA III. In the GRHDAC, temperatures up to 2000 K can be generated at high pressures by placing it in a water-cooled vacuum chamber. Temperature estimates from thermocouple measurements are within +/−35 K at the sample position up to 800 K and within +90 K between 800 and 1400 K when using a standard seat combination of cBN and WC. Isothermal compression at high temperatures can be achieved by employing a remote membrane control system. The advantage of the GRHDAC is demonstrated through the study of geophysical processes in the Earth's crust and upper mantle region. (Hwang, H., Bang, Y., Choi, J., Cynn, H., Jenei, Z., Evans, W. J., Ehnes, A., Schwark, I., Glazyrin, K., Gatta, G. D., Lotti, P., Sanloup, C., Lee, Y., & Liermann, H.-P. (2023). Graphite resistive heated diamond anvil cell for simultaneous high-pressure and high-temperature diffraction experiments. Review of Scientific Instruments, 94(8), 083903). https://doi.org/10.1063/5.013298

4-pin resistive heating cells and vacuum chamber

Mapping the electronic transitions of protonation sites in peptides using soft X-ray action spectroscopy

Near-edge X-ray absorption mass spectrometry (NEXAMS) around the nitrogen and oxygen K-edges was employed on gas-phase peptides to probe the electronic transitions related to their protonation sites, namely at basic side chains, the N-terminus and the amide oxygen.

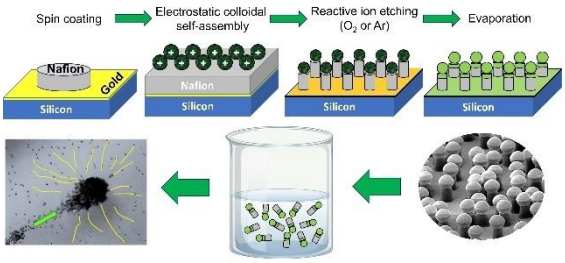


The experimental results are supported by replica exchange molecular dynamics and density-functional theory and restricted open-shell configuration interaction with single calculations to attribute the transitions responsible for the experimentally observed resonances. We studied five tailor-made glycine-based pentapeptides, where we identified the signature of the protonation site of N-terminal proline, histidine, lysine and arginine, at 406 eV, corresponding to N 1s → σ*(NH_x^+) (x = 2 or 3) transitions, depending on the peptides. We

compared the spectra of pentaglycine and triglycine to evaluate the sensitivity of NEXAMS to protomers. Separate resonances have been identified to distinguish two protomers in triglycine, the protonation site at the N-terminus at 406 eV and the protonation site at the amide oxygen characterized by a transition at 403.1 eV. (Leroux, J., Kotobi, A., Hirsch, K., Lau, T., Ortiz-Mahecha, C., Maksimov, D., Meißner, R., Oostenrijk, B., Rossi, M., Schubert, K., Timm, M., Trinter, F., Unger, I., Zamudio-Bayer, V., Schwob, L., & Bari, S. (2023). Mapping the electronic transitions of protonation sites in peptides using soft X-ray action spectroscopy. Physical Chemistry Chemical Physics, 25(37), 25603–25618). https://doi.org/10.1039/D3CP02524A

Collective motion of nafion-based micromotors in water

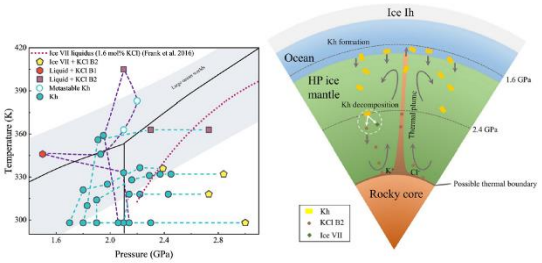
Ion exchange is one of the most interesting processes occurring at the interface between aqueous solutions and polymers, such as the well-known Nafion. If the exchanged ions have different diffusion coefficients, this interchange generates local electric fields which can be harnessed to drive fluid motion. In this work, we show how it is possible to design and fabricate self-propelling microswimmers based on Nafion, driven by ion-exchange, and fueled by innocuous salts. These Nafion micromotors are made using colloidal lithography by micro/nanostructuring Nafion in the form of asymmetric rods. These microswimmers exhibit fascinating collective motion in water driven by the interplay of their self-generated chemical/electric fields and their capability to pump matter nearby towards the collective motile structure.



The pumping activity of the microswimmers induces the formation of growing mobile clusters, whose velocity increases with size. Such dynamic structures are able to trap nearby micro/nano-objects while purifying the liquid, which acts both as the transport media and as fuel. Such phenomenology opens the door to potential applications in water remediation that are currently under development. (Fraxedas, J., Reguera, D., & Esplandiu, M. J. (2023). Collective motion of Nafion-based micromotors in water. *Faraday Discuss*). https://doi.org/10.1039/D3FD00098B

Novel high-pressure potassium chloride monohydrate and its implications for water-rich planetary bodies

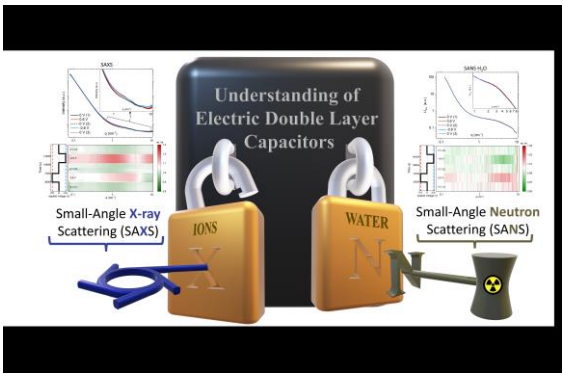
A growing body of evidence indicates that salt ions (Na^+, Ca^{2+}, Mg^{2+}, K^+, Cl^-, and SO_2^{-4}) are dissolved in water and ices of the Earth-like planets and water-rich planets. The dissolution of alkali- and alkaline earth chlorides and sulfates in water and the incorporation of salt ions in H_2O ices have a significant effect on their chemical and physical properties. Potassium chloride (KCl) is one of the most common salts in icy moons. We investigated the phase relationship of the KCl-H_2O system for different KCl concentrations at pressures of 0–4 GPa and temperatures of 298–405 K. We were able to produce a single crystal of KCl monohydrate (Kh, see figure) by adding KCl into a KCl-saturated solution and pressurizing the solution at 1.8 GPa and 298 K. Our findings reveal the existence of a novel KCl monohydrate phase with monoclinic structure, which remains stable within the pressure and temperature range of 1.6–2.4 GPa and 298–359 K. KCl monohydrate formation and decomposition may drive mantle convection in icy planetary bodies of appropriate size. (Wei, X., Zhou, Q., Li, F., Zhang, C., Sun, F., Zhang, Z., Li, R., Yu, H., Yan, Y., Li, L., Liermann, H.-P., Speziale, S., & Li, X. (2023). Novel High-Pressure Potassium Chloride Monohydrate and Its Implications for Water-Rich Planetary Bodies. Journal of Geophysical Research: Planets, 128(10), e2022JE007622). https://doi.org/10.1029/2022JE007622



Are SAXS and SANS suitable to extract information on the role of water for electric-double-layer formation at the carbon–aqueous-electrolyte interface?

This study reports on the applicability of X-ray transmission (XRT), small- and wide-angle X-ray scattering (SAXS/WAXS) and small-angle neutron scattering (SANS) for investigating fundamental processes taking place in the working electrode of an electric double-layer capacitor with 1 M RbBr aqueous electrolyte at different applied potentials. XRT and incoherent neutron scattering are employed to determine global ion- and water-concentration changes and associated charge-balancing mechanisms.

We showcase the suitability of SAXS and SANS, respectively, to get complementary information on local ion and solvent rearrangement in nanoconfinement, but also underscore the

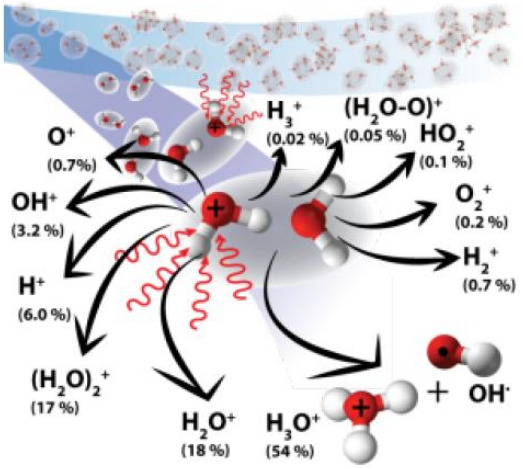


limitations of simple qualitative models, asking for more quantitative descriptions of water–water and ion–water interactions *via* detailed atomistic modelling approaches. (Seyffertitz, M., Stock, S., Rauscher, M. V., Prehal, C., Haas, S., Porcar, L., & Paris, O. (2023). Are SAXS and SANS suitable to extract information on the role of water for electric-double-layer formation at the carbon–aqueous-electrolyte interface? Faraday Discussions). https://doi.org/10.1039/D3FD00124E

Reaction pathways of water dimer following single ionization

Water dimer $(H_2O)_2$ – a vital component of the earth's atmosphere – is an important prototypical hydrogen-bonded system. It provides direct insight into fundamental chemical and biochemical processes, e.g., proton transfer and ionic supramolecular dynamics occurring in astro- and atmospheric chemistry.

We exploited a new setup, eCOMO, enabled also by CMWS funding and available for collaborative studies, providing a purified molecular beam of water dimer and multi-mass ion imaging. We report the simultaneous detection of all generated ion products of $(H_2O)_2^+$ -fragmentation following single ionization. Detailed information about ion yields and reaction energetics of 13 ion-radical pathways, 6 of which are new, of $(H_2O)_2^+$ are presented, including strong ^{18}O-isotope effects. (Vinklárek, I. S., Bromberger, H., Vadassery, N., Jin, W., Küpper, J., & Trippel, S. (2023). Reaction pathways of water dimer following single ionization (arXiv:2308.08006). arXiv). https://doi.org/10.48550/arXiv.2308.08006



ANNOUNCEMENTS

Winter Semester 2023

Seminar Series

The biweekly seminars will now be held on Thursdays at **14:00 via Zoom**. The next event is scheduled for 11th of February, 2024.

Save the date

We want to draw your attention to the next general CMWS meeting:

CMWS Water Days 2024

When: Monday 26th to Wednesday 28th of February, 2024
Where: DESY, FLASH seminar room
To register and submit your abstract please visit:
https://indico.desy.de/event/42863/

Registration will open in mid-January.
We kindly ask you to save the dates in your calendar!

Related workshops & conferences

DESY Photon Science Users' meeting

The annual DESY Photon Science Users' meeting "Research with synchrotron radiation and FELs" will take place on 24.01.-26.01.2024 in conjunction with the European XFEL Users' meeting (scheduled for 24.01.2024).

In particular, we like to draw your attention to two satellite meetings / specialized workshops, the XFEL workshop "Molecular water science" and the DESY-FLASH workshop "Community proposals using seeded operation at FLASH", which are both described in more detail below. Registration is still open.
https://indico.desy.de/event/41899/page/4731-satellite-meetings

More information about the DESY Photon Science Users´ meeting can be found here: https://indico.desy.de/event/41899/

FLASH satellite meeting "Community proposals using seeded operation at FLASH"

The Hamburg free electron laser FLASH is undergoing a significant upgrade with the FLASH2020+ project, resulting in an externally seeded FLASH1 FEL branch. The externally seeded operation at a high repetition rate, up to an effective repetition rate of 8 kHz, positions FLASH at a unique place in the international FEL landscape. The increased longitudinal coherence, spectral stability, and high average spectral flux are ideal for advanced ultrafast and nonlinear X-ray probing of matter. The upgrade will occur in 2024 and 2025. We plan to stage community-driven experiments in the time interval after commissioning, before the start of normal peer-reviewed access mode. The experiments aim to demonstrate a particular capability of the new source, which is essential for your community.

The sessions of the workshop aim to assemble the communities working together on these experiments. We are looking for 1-2 community proposals per science area (Chemistry, Materials, AMO, Biology). In all these topics, also molecular water science naturally plays an important role.

In the workshop, we will start with an introduction on the morning of Tuesday, January 23rd, followed by two parallel sessions in the morning (Chemistry, Materials) and two in the afternoon (AMO, BIO). On

Wednesday, January 24th, we will have a summary and conclusion session around lunch time.

XFEL workshop "molecular water science"

The European X-Ray Free-Electron Laser Facility (European XFEL) will open a second call for User Experiments on Molecular Water Research in the allocation period 2025-I. This call will be part of the regular 13th Call for Proposals for User Experiments with deadline in Spring 2024. Following the steps of the first successful call, will reserve an average of one week of beamtime per instrument for successful proposals. The second call shall cover an extended scope and include work on water solutions, energy/water splitting, environmental and climate research. A dedicated workshop at the EuXFEL 2024 Users Meeting will provide more information and allow for matchmaking discussions

18th International Conference on the properties of water and steam together with the 22nd symposium on thermophysical properties

The combined 18th International Conference on the Properties of Water and Steam (ICPWS) is focused on the properties, science, and applications of water, steam and aqueous systems, primarily as needed for the electric power generation community and within climate science. The Symposium is concerned with theoretical, experimental, simulation, and applied aspects of the thermophysical properties of gases, liquids, and solids, including biological systems.

18th International Conference on the properties of water and steam together with the 22nd Symposium on thermophysical properties

When: June 23rd to 28th, 2024
Where: Boulder, CO, USA
Website:
https://www.thermosymposium.org/

Double layer reloaded: theory meets experiment Symposium

The symposium will focus on an improved understanding of the structure, dynamics, and properties of the electrode-electrolyte interface on the molecular scale. It aims at bringing together experimentalists and theoreticians to foster the development of a unified microscopic picture of the electrochemical interface. It will specifically address the structure and dynamics of interfacial water and ions in the electrolyte solution near the electrode surface, the electronic structure and potential distribution at the interface, and the effect of the interface structure on the electrochemical reactivity.

Double layer reloaded: theory meets experiment Symposium

Within the 75th Annual Meeting of the International Society of Electrochemistry.

When: August 18th to August 23rd, 2024
Where: Montréal, Québec, Canada

For further information please contact
magnussen@email.uni-kiel.de
or visit
https://annual75.ise-online.org/symposia.php#s13

CAREER & OPEN POSITIONS

The CFEL Controlled Molecule Imaging group at DESY and UHH has several fully funded openings for doctoral students related to molecular water science:

Laser-induced electron diffraction of thermal-energy ultrafast (bio)chemical dynamics

You will use laser-induced electron diffraction to image the ultrafast elementary steps of chemical dynamics of "everyday (bio)chemistry", at thermal-energy scales similar to room temperature, with atomic resolution. The research builds on cutting-edge controlled-solvated-molecule preparation and imaging techniques available in our group our

experience with ultrafast lasers. It is in close connection with the Theory team of our group and collaboration partners in Hamburg and elsewhere. This project is part of the federal cluster of excellence Center for Ultrafast Imaging.

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

Cryogenically cooled and controlled beams of proteins for single-particle diffractive imaging

You will work on novel sample preparation and control concepts for structural biology at x-ray free-electron lasers (XFELs). You will implement and advance techniques to shock-freeze solvated biological macromolecules to image and characterize these samples, to implement control techniques such as species selection and laser alignment, and to exploit the controlled biomolecular samples in single-particle diffractive-imaging experiments at x-ray free-electron lasers. This work focuses on developing and implementing experimental methodology that allows for the spatial separation of macromolecular conformers in sample-injection pipelines for XFEL experiments.

Ultrafast light-induced dynamics of model chromophores in size-controlled water clusters

You will study the ultrafast light-induced dynamics of model chromophores in size-controlled water clusters to investigate how different-sized chromophore-water clusters can be separated to examine the influence of successive water molecule additions on the dynamics of biologically relevant systems. The research builds on and advances the cutting-edge solvated-molecule preparation and imaging techniques available in our group and our collaborators' experience with ultrafast lasers. This project is part of the Röntgen-Angstrom-Cluster project UDIET in close collaboration with Francesca Calegari in Hamburg and partners in Lund, i.e., Per Johnson and Mathieu Gisselbrecht.

Investigating solvent effects in the dynamics of biologically relevant model systems

You will study the ultrafast light-induced dynamics of microsolvated biologically relevant molecules, such as DNA bases or amino acids, in the gas phase. Protective mechanisms through the omnipresent fluid environment on biological matter will be modelled and examined. 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 is in close collaboration with Francesca Calegari in Hamburg and our partners Per Johnson and Mathieu Gisselbrecht in Lund.

We cordially invite you to announce your open positions here!

PEOPLE IN THE COMMUNITY

In this edition, we have had the privilege of interviewing Fivos Perakis from Stockholm University, Yongjae Lee from Yonsei University, and Gavriel Arbiv from KU Leuven. Meet them in the interviews below and get some ideas about their views on science, molecular water and life.

Fivos Perakis

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

Fivos: I got into molecular water research by accident. I initially started my PhD on a different topic, related to solar cells in collaboration with a group in another university. However, after one year of work, my supervisor and I realized that the results did not make much sense and after discussions with the collaborators, that this approach was not working actually. At this stage, my supervisor suggested to switch topics and look into water. I was surprised by his suggestion, because I thought that everything was known by now about water. Little did I know that this was only the beginning of a long interesting trip down the rabbit hole of the mysteries of water.

Please tell us about your latest research project.

Fivos: In my group we investigate the structural dynamics of water and its role as a solvent around small organic molecules and proteins. We explore the two-liquid hypothesis in water, e.g. that water can exist in two liquid forms of different density in deeply supercooled regime. Therefore, our experiments explore cryogenic conditions, since this regime can also have relevant applications in understanding how cryoprotectant can suppress freezing and practical implications in the cryostorage of biological solvents. We mainly perform measurements at large-scale facilities, such as X-ray synchrotrons and X-ray free electron lasers (XFELs) for probing dynamics of water at various lengthscales using techniques such as X-ray Photon Correlation Spectroscopy (XPCS) and time-resolved X-ray scattering.

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

Fivos: Resolving the hypothesized liquid-liquid critical point is an open question in fundamental molecular water research. Even though this is the cornerstone of the two liquid hypothesis, its existence has not been verified experimentally. In addition, from a more applied perspective, I think that we need to apply this understanding to improving water cleaning and desalination technologies. This is an important challenge for humanity and we need new greener and more economic approaches, such as for example cryo-desalination, which for the time being is still too energy-intensive. Finally, one of the most important unexplored aspects I believe is related to the role of water in life processes. Even though there is a lot of work done on the biological hydration of water, e.g. water in the direct proximity of biomolecules, it is still unknown how collective effects in water can influence activity in the cell, for example by hydrodynamic flows and fluctuations.

If you could wish for a collaboration partner for your current research - what specific expertise or knowledge would this partner ideally contribute to the topic?

Fivos: It would be interesting to collaborate with someone who knows more about water cleaning and desalination approaches from a material science perspective. In my group, we specialize in characterization techniques, so that would make a good combination. Also, even though I am mainly doing experimental work, I also like to work with molecular dynamic simulations. I would like to find a collaboration partner with knowledge of large-scale molecular simulation from whom I can learn from, since this is an exciting area for simulating phenomena like liquid-liquid phase separation and crystallization.

What was the most important advice someone gave you?

Fivos: One of the most important advice I received during my postdoc years at Stanford was to be strong and believe in my ideas. There will always be people out there who will tell you that "this is impossible" or "that won't work". It is important to learn to trust yourself and not be afraid to stick your neck out and stand up for your vision.

When do you have your best ideas?

Fivos; Usually new ideas come to me at random moments, often when I am on the move. For example, it can be when riding the bike home from work or during a long flight when I am looking out the window. When ideas come up like that have a fresher feel, than when sitting in a usual setting like in my office. I also enjoy coming up with ideas when brainstorming with my team or collaborators, since this collective thinking can stimulate really interesting results.

What does make you laugh?

Fivos: My son makes me laugh and brightens my day. I also find myself laughing loudly when listening to audio books in public transport. One of my colleagues also commented that during group meetings, our laughter echoes down the hallway. I am grateful for my group members, since we can have quite a lot of fun even when discussing science!

How do you balance your professional and personal life?

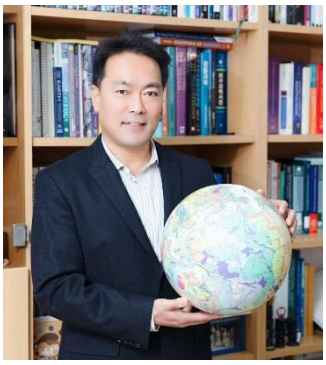
Fivos: I aim to be as organized as possible, when it comes to my routines and tasks, so that I minimize the effort required. Having flexibility in the schedule provided by an academic environment also helps. I typically spend most weekends with my family, unless I have to travel for work or something urgent comes up, and make sure to take all of my vacation days, while trying to not work during those.

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

Fivos: In my free time I enjoy spending time with my family in nature, either hiking or biking in the forest or swimming at the lake near my place. I also love travelling to visit our families abroad and usually spend the summers next to the seaside.

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

Fivos: When doing research focus on the process itself and enjoy both the creative aspects and its challenges. If you really enjoy this process, it can lead you to a new and interesting place both scientifically and career-wise.



Yongjae Lee

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

Yongjae: During my Ph.D., I studied how water can be released from water-containing minerals such as zeolites. Usually, *heat* is required for water to be released from its confining crystalline matrix, and I observed structural changes associated with water release. After my Ph.D., I started to investigate the opposite behavior of water insertion into crystalline matrix and found that *pressure* can be the key to open certain host matrix to make it accommodate (more) water. For the Earth, water release and insertion occurring in minerals could mean a lot to make our world a dynamic and habitable planet. There is lots of water around us, mainly in the vast oceans covering about 70% of the Earth's surface. Even the most conservative estimate, however, expects that more water is stored inside the planet, in the mantle and maybe even in the core (in the form of hydrogen and oxygen). Therefore, how water can be transported, released, and interact with various components of the Earth would be, by itself, translated to how this planet became habitable in the form that we can live on.

Please tell us about your latest research project.

Yongjae: Water transport into the Earth's interior starts from subduction, a global process of old and cold components of lithospheric plate sinking into the mantle. The current estimate says that about 10^8 Tg of water enters through globally distributed subduction zones per million years. It is those water-containing minerals that carry water into the Earth. As water-containing minerals subduct deep down to about 200 km depth, they generally release water as temperature increases, together with pressure, which causes earthquakes and volcanism. My current research interest lies on discovering its opposite behavior as certain class of water-containing minerals were shown to uptake more water, instead of releasing them, as we named 'super-hydration' or 'hydration breakdown' in the literature. This would then mean that even more water has been transported into the Earth over the vastly long years of the Earth's history.

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

Yongjae: Subduction is a relatively well-studied field where petrologists, geochemists, seismologists, and mineralogists like myself, work closely in competitive as well as collaborative manners. However, for the deeper interior of the Earth from the lower mantle, i.e., about 660 km depth, down to the core-mantle boundary, i.e., about 2900 km depth, much has yet to be discovered, especially in terms of water transportation scheme.

In our recent work, we assumed about 1% efficiency of surface water touching down the core-mantle boundary. The reaction between water and iron at the core-mantle boundary conditions led to a chemical exchange to form a stable hydrogen-rich layer in the topmost outer core, providing a possible origin on the putative E' layer. In the near future, I also wish to study the fate of water on Mars as it is believed there were once oceans, rivers, and lakes on the surface of Mars.

If you could wish for a collaboration partner for your current research - what specific expertise or knowledge would this partner ideally contribute to the topic?

Yongjae:: As an experimental mineralogist, I wish to interact with people in geochemistry and geodynamics, who can provide guidance and confirmation on our experimental findings. This doesn't mean that I am not interested in interacting with people outside my narrow discipline as I often find much insights from seemingly unrelated people.

What was the most important advice someone gave you?

Yongjae: There is a famous wise saying in Korea, "Let gold be like a stone". As we study minerals to understand the Earth and other planets, it could be reversed to "Let a stone be like gold".

When do you have your best ideas?

Yongjae: Ironically, it is always when I leave my desk when I get to think of things I haven't thought of.

What does make you laugh?

Yongjae: My son and daughter…and more or less, my wife as well…

How do you balance your professional and personal life?

Yongjae: I hope they are not separate as I sometimes find myself in my office during weekends and holidays.

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

Yongjae: I am realizing as I get interviewed that I was always doing *water-related research*. Water out of or into minerals or their interactions.

Recently, I happened to visit a porcelain artist who tries to reproduce the famous Korean celadon. I was shocked to see the artist controlling the subtle interaction between pottery material and fluid latex at temperatures over 1200 degree Celsius. This is the mineral-water interaction implemented into the art. I am thinking of such *water-related art* after my future retirement.

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

Yongjae: Water is special in every aspect. It is ubiquitous yet very powerful. Water affects almost everything on the planet from the surface to the interior. Doing water-related research in any field should be regarded as a special privilege as water is always hiding something to be discovered by you.

Gavriel Arbiv

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

Gavriel: I have always been fascinated by the infinite properties of this small molecule. I come from physical chemistry, and my master's topic was catalysis. When I was about to finish, I wanted to expose myself to other fields, and I found a project (WaTuSo) that aimed at sustainability and offered something that sounded like a dream for a chemist, which I hope I can fulfill.

Please tell us about your latest research project.

Gavriel: I'm using NMR to follow and monitor the water behavior. Tens of papers were written about how much knowledge you can reach from the signal you receive. We developed a new method that calibrates the NMR probe-head for dielectric measurements, and by that, I added another spectroscopy in-situ to our measurements.

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

Gavriel: I am following confined water and the change in the dielectric properties. I would like to correlate it with the evolution of a droplet and eventually change its properties.

If you could wish for a collaboration partner for your current research - what specific expertise or knowledge would this partner ideally contribute to the topic?

Gavriel: I would like to combine my scientific knowledge with someone from a more artistic field, for instance, a product designer.

What was the most important advice someone gave you?

Gavriel: It is not easy to point out one, but I think the most beneficial advice I use these days is to split every big challenge into many small ones.

When do you have your best ideas?

Gavriel: While running or when I am explaining to someone out of the field

What does make you laugh?

My dad jokes.

How do you balance your professional and personal life?

Gavriel: I have some friends who are not related to my field. But I am a Ph.D. student, so there is no personal life besides sleeping.

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

Gavriel: Doing beer-related research.

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

Gavriel: Accept that your energy and motivation are depressible assets, so use it wisely.

CONFERENCES & WORKSHOPS OVERVIEW

2024

XFEL workshop on molecular water science
January 23, 2024. Schenefeld, Germany
https://indico.desy.de/event/42730/

DESY Photon Science Users´ Meeting
January 25-26, 2024. Hamburg, Germany
https://indico.desy.de/event/41899/

CMWS Water Days 2024
February 26-28, 2024. Hamburg, Germany
https://indico.desy.de/event/42863/registrations/5902/

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)

Water and Aqueous Solutions (GRC)
July 21-26, 2024. Holderness, NH, United States
2024 Water and Aqueous Solutions Conference (Gordon Research Conference)

EMLG–JMLG Annual Meeting 2024
September 8-13, 2024. Trieste, Italy
Structure and Dynamics of Hydrogen-bonded Liquid Systems

Liquid Matter Conference 2024
September 22–27, 2024. Mainz, Germany
12th Liquid Matter Conference

-SAVE THE DATE-