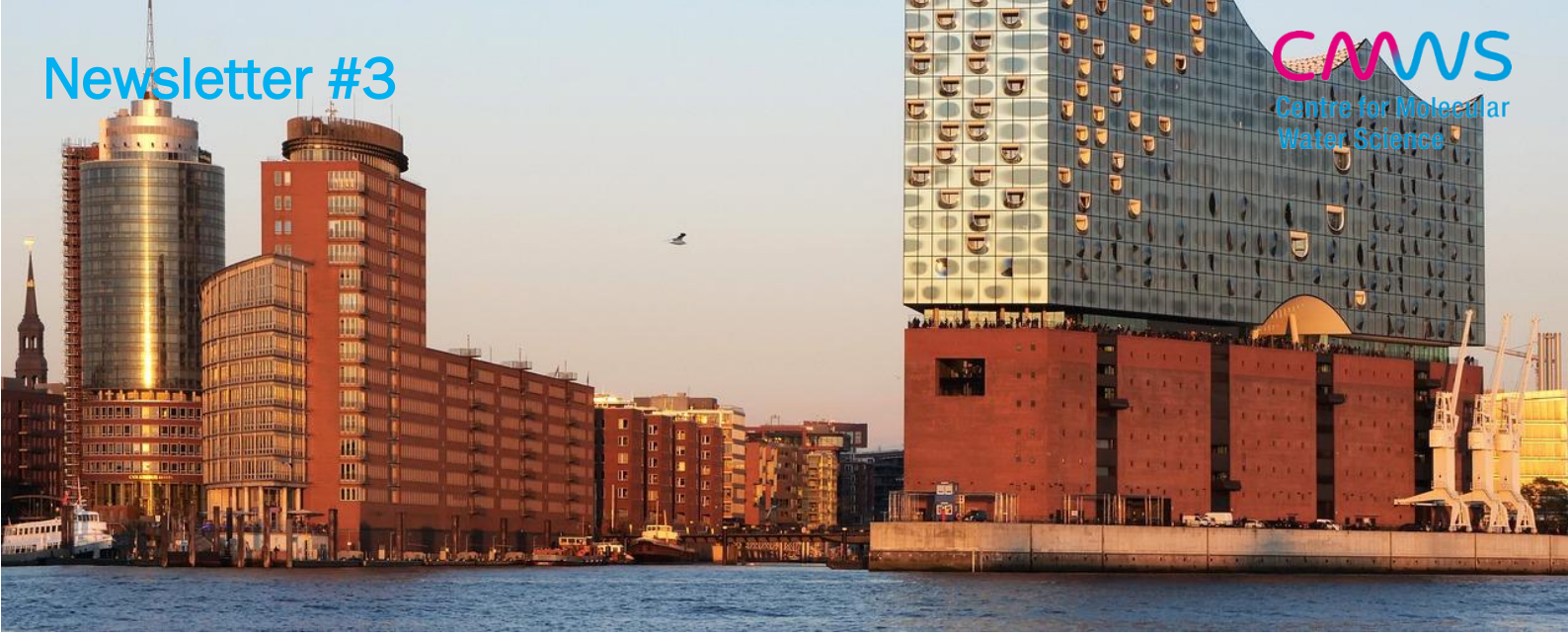
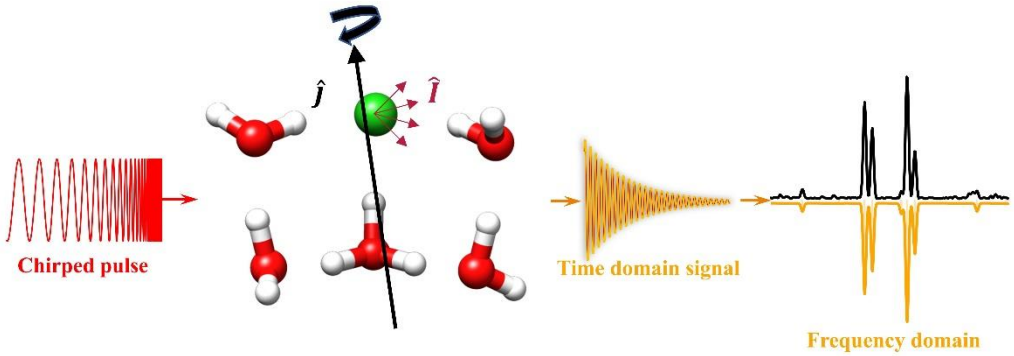
Newsletter #3





Hydrogen chloride (HCl) spontanously dissociates within a hydrogen-bonding network of five water molecules. This is probed by measuring the coupling of the chlorine nuclear spin with the rotational angular momentum of the cluster. F. Xie, D.S. Tikhonov, M. Schnell, Electric nuclear quadrupole coupling reveals dissociation of HCl with a few water molecules, Science 384 (2024) 1435-1440. https://doi.org/10.1126/science.ado7049

Dear CMWS colleagues,

Three editions make a tradition, and with this, we are happy to share the next CMWS newsletter with you. You will find again some latest research and people news, an introduction to the CMWS infrastructure eCOMO, a mobile endstation designed for conducting controlled-molecule experiments, interviews with CMWS colleagues as well as save-the-date announcements.

Furthermore, we are happy to share with you that 47 partner universities and institutions signed the common CMWS declaration. We are planning an inauguration and kick-off ceremony during next year's CMWS Water Days, which will take place on February 25th-27th, 2025. Please save the date! Of course, we plan to again have an interesting line up of invited and contributed talks during the Water Days. As always, we are open for suggestions, also if you have ideas for a specific workshop.

The CMWS declaration also comes with a slim governance, and in the course of establishing it, each research pillar will have to elect speakers – two per pillar, one main speaker and one vice speaker. We will start this process soon, so please think whether you would consider yourself to run for this exciting position. The pillar speakers will be elected by the scientists of the respective pillars. Concerning the role of the pillar speakers: In short, they are the first contact points for scientific and organizational requests and are supposed to actively steer the scientific program – for example in the form of organizing workshops to foster exchange within and between the pillars, to promote networking, and to encourage and support funding acquisition activities. They will be members of the management board of the CMWS to help steer CMWS activities and are encouraged to get involved in the organization of the CMWS Water Days.

Last but not least, we would like to inform you about the current status of the application for funding from the Helmholtz association to extend the CMWS research infrastructure, including a research building on the DESY site. While we were initially planning to submit the application this summer, it needed to get postponed, and we are currently in the process of identifying the best suited submission timeline. We will keep you posted!

As always, feedback to this newsletter and suggestions for CMWS activities in general are very welcome.

With warm regards,

The CMWS team.

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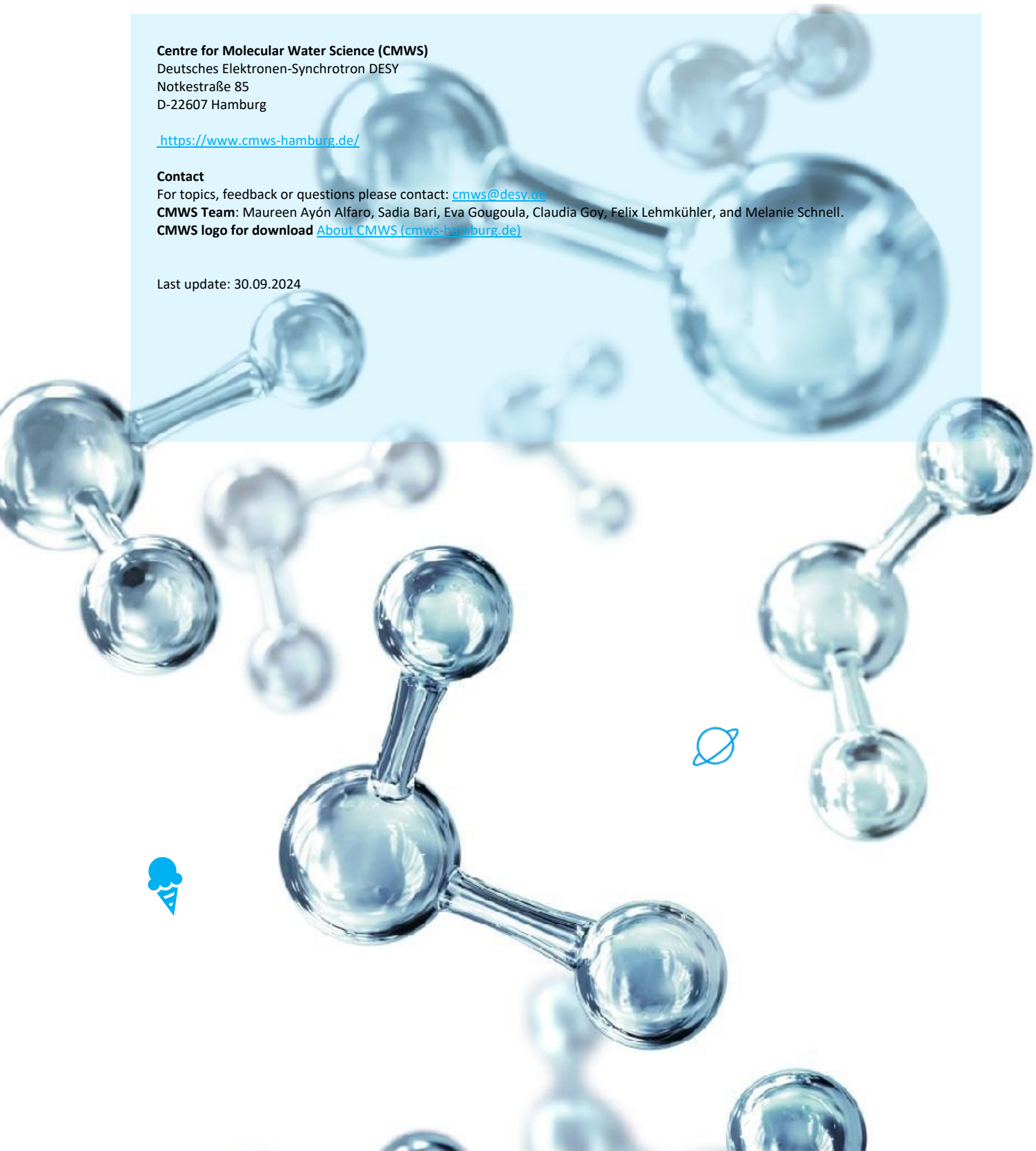
CMWS logo for download About CMWS (cmws-hamburg.de)

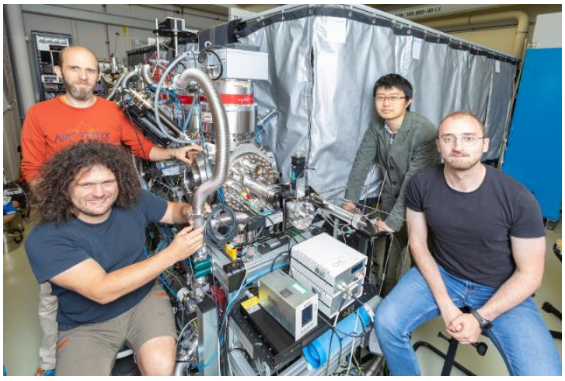
Last update: 30.09.2024



INSIDE CMWS

Dedicated CMWS infrastructure: A mobile endstation for controlled molecule experiments (eCOMO)

A new versatile transportable endstation for controlled-molecule (eCOMO) experiments was put into operation in DESY's CFEL Controlled Molecule Imaging group (CMI) of Jochen Küpper in a collaborative CMWS project with the ATTO group of Francesca Calegari.



Sebastian Trippel (front left) and Ivo Vinklárek (front right), with Wuwei Jin and Hubertus Bromberger in the background, in front of the eCOMO endstation in the CMI laboratory.@CMI.

The eCOMO setup provides a unique combination of molecular-beam purification by electrostatic deflection and simultaneous ion and electron momentum detection by velocity-map imaging (VMI). The b-type electrostatic deflector enables the spatial separation of species based on their effective-dipole-moment-to-mass ratio, enabling the selective study of molecular ensembles in individual rotational quantum states, conformational structures, or molecular-cluster species, including microsolvated molecules. The double-sided VMI spectrometer equipped with two high-temporal-resolution event-driven Timepix3 cameras, operated with our public pymepix software, allows highly parallel detection of all product ions and electrons. The setup was commissioned and characterized in first experiments on carbonyl sulfide (OCS), and further studies on water-containing clusters were performed already.
eCOMO enables ultrafast-dynamics studies at a wide range of light-source facilities, from table-top to free-electron lasers, making it suitable for research activities spanning atomic, molecular, and cluster physics with applications in chemistry, material science, energy science, and structural biology. This particularly includes light-induced dynamics studies of microsolvated biomolecules such as nucleobases and model chromophores – with a well-defined number of water molecules attached to the molecules – to investigate the influence of the local water environment.
A scientific publication on the endstation is in preparation.
For further information see, here.

Christina M. Tonauer receives the Georg-and-Christine-Sosnovsky Prize 2024

Christina M. Tonauer (DESY/ U Innsbruck) receives the Georg-and-Christine-Sosnovsky Prize 2024 for her dissertation "Near-Infrared Spectroscopy for Characterization of Crystalline and Amorphous Ices", performed at the University of Innsbruck and as part of a DESY Early Science Project where she first-time characterized 11 phases of ice in the wavelength range 1-2.5 µm. Her work establishes the previously neglected near-infrared range as a significant spectral region for the detection and identification of various ice structures in space, thereby enabling fundamental insights into the composition of icy

Prof. Thomas Loerting and Christina Tonauer. Photo credit: Universität Innsbruck.

celestial bodies through space telescopes such as the James Webb Space Telescope JWST or JUICE. Congratulations, Christina!

Topical proposal calls on molecular water science.

Successful proposal call for molecular water science at PETRA III

In the framework of the second targeted challenge-driven (TCD) proposal call on Molecular Water Science 2024 at the X-ray synchrotron PETRA III, two proposals have received beamtimes, both with strong contributions from CMWS researchers. Overall, the proposals have received experiment time for more than 20 beamtimes at five different beamlines of PETRA III for the next two years. In one of the projects, transport phenomena and dynamics of aqueous electrolytes in nanoporous confinement will be studied as a collaboration of CMWS researchers from University Leoben (Austria), TU Hamburg, Forschungszentrum Jülich, and University of Hamburg. The researchers will use static and time-resolved scattering methods as well as nanotomography to investigate the properties of confined solutions.

The other successful project is focused on spectroscopy and scattering experiments revealing the formation process of clathrate hydrates in different environments. Scientists located at DESY, KU Leuven (Belgium), TU Dortmund, University of Saskatchewan (Canada), and Stockholm University will contribute to these experimental campaigns. Together with the experiments from the first TCD call 2022, more than 120 days of beamtime will have been dedicated within this new proposal type.

Proposal call at the European EXFEL

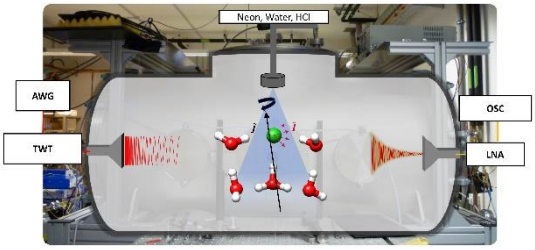
Based on the evaluation of the first call on Molecular Water Science and the feedback from the user community, European XFEL decided to open also a second call for User Experiments on Molecular Water Science in the allocation period 2025-I. This call was part of the regular 13th Call for Proposals for User Experiments with deadline in Spring 2024. Building on the outcomes of the first call, an average of one beamtime slot per instrument was reserved for successful proposals. The second call was to cover an extended scope and accept also proposals on water solutions, energy/water splitting, environmental and climate research.

Furthermore, collaborations (joint proposals) between expert groups and newcomers were encouraged. A total of 25 proposals was received, requesting beamtime at all six operational instruments. The outcome of the evaluation will be announced soon.

HIGHLIGHTS & RESEARCH

Electric nuclear quadrupole coupling reveals dissociation of HCl with a few water molecules

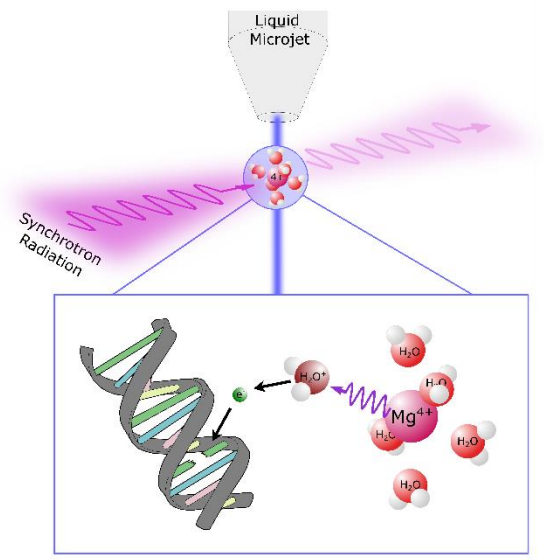
Investigating the dissociation of acids in the presence of a limited number of water molecules is crucial for understanding various elementary chemical processes. In our study focusing on HCl $(H_2O)_n$ clusters formed in a cold and isolated jet



expansion, we utilized the nuclear quadrupole coupling tensor obtained via rotational spectroscopy to decipher the nature of the H-Cl chemical bond in a micro-aqueous environment. For n = 1 to 4, the H-Cl bond is covalent. At n = 5 and 7, the contact ion pair of $H_3O^+Cl^-$ is spontaneously formed within the hydrogen bond networks of "book" and "cube" acid-water clusters, respectively. (F. Xie, D.S. Tikhonov, M. Schnell, Electric nuclear quadrupole coupling reveals dissociation of HCl with a few water molecules, Science 384 (2024) 1435 - 1440. *https://doi.org/10.1126/science.ado7049).*

X-ray radiation damage cycle of solvated inorganic ions

X-ray-induced damage is one of the key topics in radiation chemistry. Experimental investigations on photochemistry on a molecular level are challenging in realistic environments, e.g., liquid phase, due to the high vacuum requirements for charged particle spectroscopy. We apply multi-electron coincidence spectroscopy to X-ray-irradiated aqueous solutions of inorganic ions to investigate the production of low-energy electrons (LEEs) in a predicted cascade of intermolecular charge- and energy-transfer processes, namely electron-transfer-mediated decay (ETMD) and interatomic/intermolecular Coulombic decay (ICD). The advanced coincidence technique allows us to identify several LEE-producing steps during the decay of 1s vacancies in solvated Mg^{2+} ions, which escaped observation in previous non-coincident experiments. We provide strong evidence for the predicted recovering of the ion's initial state. In natural environments, the recovering of the ion's initial state is expected to cause inorganic ions to be radiation damage hot spots, repeatedly producing destructive particles under continuous irradiation. We provide an important progress towards the exploration of radiation damage in the liquid phase as well as insight into the role of the water environment for solutes exposed to X-rays.

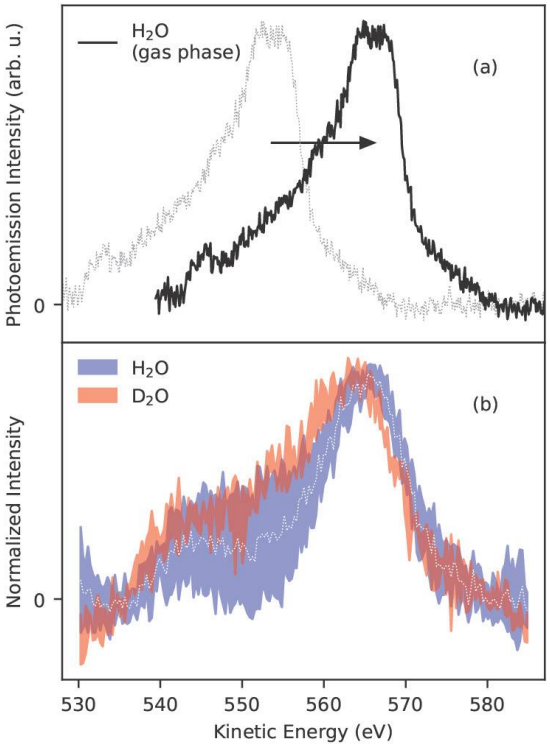


The project became possible through the cooperation of several CMWS partners and benefited from the scientific exchange within CMWS. (D. Bloß, F. Trinter, I. Unger, C. Zindel, C. Honisch, J. Viehmann, N. Kiefer, L. Marder, C. Küstner-Wetekam, E. Heikura, L.S. Cederbaum, O. Björneholm, U. Hergenhahn, A. Ehresmann, A. Hans, X-ray radiation damage cycle of solvated inorganic ions, Nat Commun 15 (2024) 4594. https://doi.org/10.1038/s41467-024-48687-2)

Water: molecular origins of its anomalies

We present a combined experimental and theoretical investigation of the radiationless decay spectrum of an O 1s double core hole in liquid water. Our experiments were carried out using liquid-jet electron spectroscopy from cylindrical microjets of normal and deuterated water. The

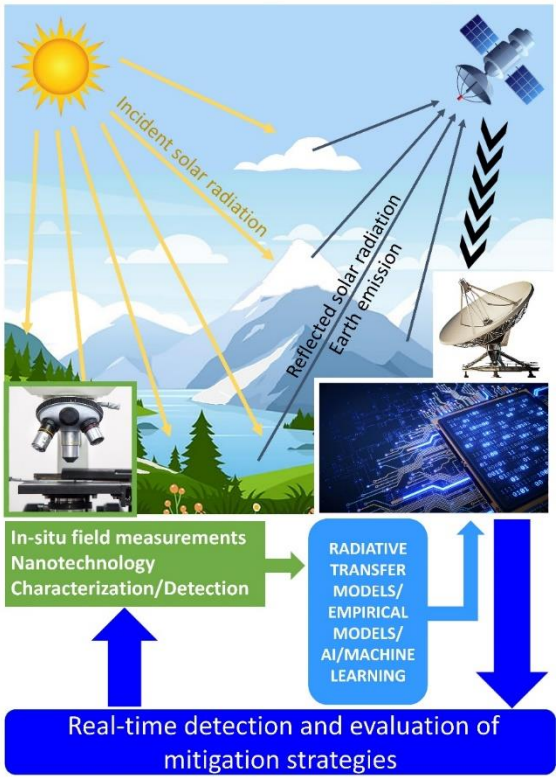
signal of the double-core-hole spectral fingerprints (hypersatellites) of liquid water is clearly identified, with an intensity ratio to Auger decay of singly charged O 1s of 0.0014(5). We observe a significant isotope effect between liquid H_2O and D_2O. For theoretical modeling, the Auger electron spectrum of the central water molecule in a water pentamer was calculated using an electronic-structure toolkit combined with molecular-dynamics simulations to capture the influence of molecular rearrangement within the ultrashort lifetime of the double core hole. We obtained the static and dynamic Auger spectra for H_2O, $(H_2O)_5$, D_2O, and $(D_2O)_5$, instantaneous Auger spectra at selected times after



core-level ionization, and the symmetrized oxygen-hydrogen distance as a function of time after double core ionization for all four prototypical systems. We consider this observation of liquid-water double core holes as a new tool to study ultrafast nuclear dynamics. This work was performed in a collaboration of CMWS researchers, in particular from Pillar IV -- Real-time Chemical Dynamics. (Trinter et al. Water: Molecular Origins of its Anomalies, AIP Publishing (n.d.). *https://pubs.aip.org/collection/20468/Water-Molecular-Origins-of-its-Anomalies* (accessed July 12, 2024).

Bringing satellite and nanotechnologies together: unifying strengths against pollution and climate change

Despite the tremendous length scale gap between satellite and nanotechnologies, their combination could create unprecedented synergy to monitor, remediate and protect our planet's ecosystem against increasing environmental contamination. Satellites are essential for identifying and monitoring large-scale pollution in water and ice, assessing land degradation, and examining ocean health with high spatial and temporal resolution. Meanwhile, nanotechnology exploits the unique

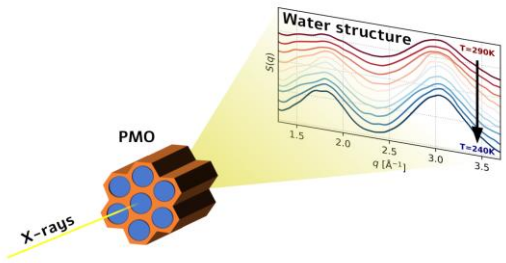


properties of sub-micron materials, enabling sensitive/selective sensors and efficient contaminant capture/degradation, while advanced nanocharacterization and nanofabrication offer deeper insights/quantification at the nanoscale, and precise design of functional nano-devices. The cross-talk between both fields can (i) boost low-cost picosatellite development, expanding miniaturization and creating novel compact and lightweight components, (ii) refine satellite information retrieval models and validation tools

for environmental indicators, using high quality on-ground experimental inputs of targets with nanocharacterization tools and ground nanosensors, (iii) refine retrieval models with theoretical inputs from nanoscience to get insights into light/micro-nanoparticulate interactions, (iv) improve pollution assessment, source identification, and contaminant transport, aiding targeted remediation and surveillance, and (v) create accurate geospatial data/maps for environmental quality indicators to support scientific evidence and influence environmental protection decisions. Activity in this field would perfectly match the CMWS strategic research pillar Water in Climate-, Astro-, and GeoSciences. (A. Ferral, M. Bonansea, C.M. Scavuzzo, F. Nemiña, M. Burgos Paci, J.C. Ramirez, B. Sepúlveda, J. Fraxedas, M.J. Esplandiu, Bringing satellite and nanotechnologies together: unifying strengths against pollution and climate change, Front. Nanotechnol. 6 (2024). *https://doi.org/10.3389/fnano.2024.1332820).*

Structure of water under confinement in periodic mesoporous organosilicas investigated by X-ray scattering

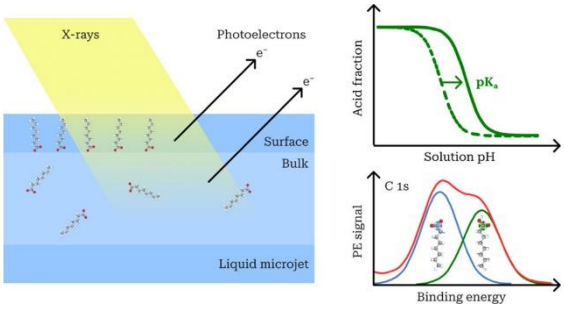
In our recent study, the effect of pore wall chemistry and pore diameter on the structure of confined water in nanometer-sized pores of periodic mesoporous organosilicas (PMOs) was studied by X-ray scattering. A shift in the first structure factor peak at q ≈ 1.8 $Å^{-1}$ reveals a variation in the density of the confined water in dependence of hydrophilicity and pore size. Smaller and more hydrophilic pores induce a lower density in the water. The running coordination numbers suggest that smaller and more hydrophilic confinement leads to a stronger developed tetrahedral network in confined water, while confinement in larger and hydrophobic pores give tetrahedral arrangements that are bulk-like or even



less pronounced than in bulk water. These investigations were followed up by a study, where the structure and orientation of ice in PMOs was investigated, (in print in J. Chem. Phys. (DOI: 10.1063/5.0216697)). The studies were carried out as a collaboration of CMWS partners at DESY and University Hamburg in the framework of the state funded research project LFF-FV68 and was also supported by CMWS through an Early Science Project. (N.C. Gießelmann, P. Lenz, S.-M. Meinert, T. Simon, W. Jo, N.N. Striker, M. Fröba, F. Lehmkühler, Structure of Water under Confinement in Periodic Mesoporous Organosilicas Investigated by X-ray Scattering, J. Phys. Chem. C 128 (2024) 499–507. *https://doi.org/10.1021/acs.jpcc.3c0649).*

Surfaces of atmospheric droplet models probed with synchrotron XPS on a liquid microjet

Water and a myriad of other chemical species are present in Earth's atmosphere in all basic forms of matter. Suspended nano- and microscopic aerosol particles and cloud droplets play crucial roles in regulating climate, formation of air pollution, and transmission of communal diseases. Interactions of aerosols and droplets with water are key to these

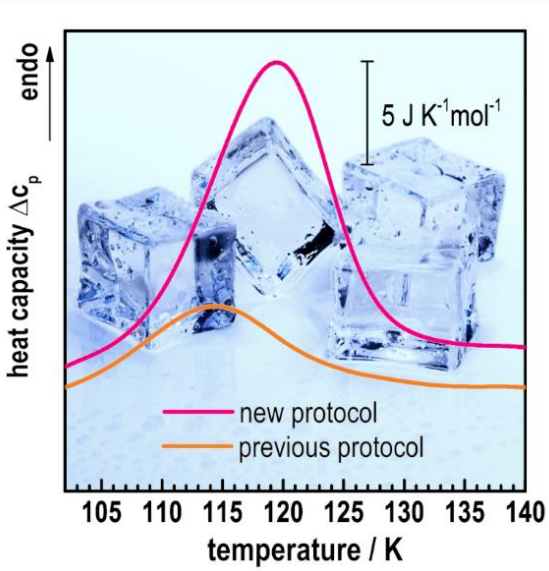


effects, but challenging to quantify. Surfaces are a prominent part of aerosols and droplets, due to their high surface area to bulk volume ratios. Many atmospheric compounds are surface-active, leading to enhanced surface concentrations in aqueous solutions, and display Brønsted acid-base character. We used synchrotron X-ray photoelectron spectroscopy to obtain direct molecular-level information on the surface composition and structure of aqueous solutions of surface-active organics as model systems for atmospheric aerosol and cloud droplets. The alkyl and hydrophilic groups of atmospheric carboxylic acids, alkyl-amines, and their conjugate acids and bases were identified

from core-level C 1s and N 1s signals. For each pair, the protonation equilibrium was significantly shifted toward the neutral form in the surface, compared to the bulk solution, across the full pH range. This apparent shift of acidity in the surface may be toward either higher or lower pH, depending on whether the acid or base form of the pair is the neutral species. The surface shifts are broadly consistent with the relative differences in surface activity of the individual acid and base conjugates in aqueous solutions. These surface-specific effects may profoundly influence atmospheric chemistry mediated by aqueous aerosols and cloud droplets, but are currently not taken into account in atmospheric models. (N.L. Prisle, Surfaces of Atmospheric Droplet Models Probed with Synchrotron XPS on a Liquid Microjet, Acc. Chem. Res. 57 (2024) 177–187. *https://doi.org/10.1021/acs.accounts.3c00201).*

Near-infrared spectroscopy for remote sensing of porosity, density and cubicity of crystalline and amorphous H_2O Ices in astrophysical environment

Water's phase diagram shows several pairs of ices with virtually the same oxygen network but a different – either "ordered" or "disordered"-hydrogen network. These subtle structural differences have profound consequences on macroscopic material properties like plastic flow or permittivity. At low temperatures, H-ordering is thermodynamically favored but often geometrically frustrated. This is especially true for D_2O ices, which are key for structure determination by neutron diffraction. In our study based on the deuterated ice XII-XIV pair [C.M. Tonauer, E. Hauschild, S. Eisendle, V. Fuentes-Landete, K. Yamashita, L. Hoffmann, R. Böhmer, T. Loerting, Strategies to obtain Highly Ordered Deuterated Ices presented on the Example of Ice XIV, PNAS Nexus 2 (2023), pgad418. https://doi.org/10.1093/pnasnexus/pgad418] we present new experimental strategies for overcoming geometric frustration of ordering, thereby tripling levels of order relative to literature studies (**Fig. 1**), which opens up new possibilities for exploring water's phase diagram and studying properties of icy bodies. In a second study arising from the joint CMWS science project between

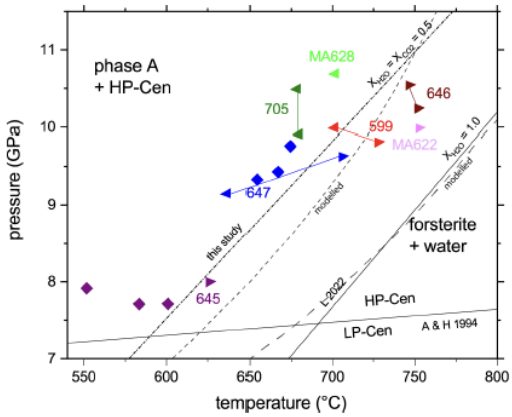


Thermograms unveiling a tripling of order by employing the new experimental protocol

University of Innsbruck and DESY, we provide reference spectra of crystalline and amorphous ices in the near-infrared, allowing for remotely accessing properties of icy moons, cometary ice or Saturn rings by telescopes like the James Webb Space Telescope. (C. M. Tonauer, E.M. Köck, R. Henn, J.N. Stern, L. del Rosso, M. Celli, C. Kappacher, S. Leiter, C.G. Kirchler, C. W. Huck, T. Loerting, Near-infrared Spectroscopy for Remote Sensing of Porosity, Density and Cubicity of Crystalline and Amorphous H_2O Ices in Astrophysical Environments, Astrophys. J. (accepted)) *https://doi.org/10.3847/1538-4357/ad4f82.*

In situ study of the reaction phase A plus high-P clinoenstatite to forsterite plus water at reduced water activity

Understanding the role of water in the dynamics of the Earth's interior is one of the key challenges in the CMWS. Molecular water is cycled from the surface of our planet to the deep Earth where it is stored in hydrous minerals such as phase A, $Mg_7Si_2O_8(OH)_6$ and where its release at specific P-, T- conditions may induce partial melting, volcanism and earthquakes. We examined such a release of water by the reaction of phase A plus enstatite to forsterite by means of in situ X ray diffraction measurements with the large-volume press at the synchrotron PETRA III, Hamburg. To mimic more realistic conditions, the experiments were performed under



reduced water activity (a_{H2O}<1). Compared to results under water-saturated conditions the P-, T-coordinates of this reaction are shifted by about 100 °C to lower temperature. Thus, even at a water activity below 1 this dehydration reaction can occur in the deep Earth if only in cold subduction environments. The newly formed dehydration product forsterite was of nanometer size, and it is discussed that such fine-grained reaction products could initiate seismicity due to mechanically-induced instabilities. (Lathe, C., Koch-Müller, M., Wunder B., Appelt,O., Sieber M., Bhat S., Farla, R. In situ study of the reaction phase A plus high–P clinoenstatite to forsterite plus water at reduced water-activity. European Journal Mineralogy, 35, (2023) 1149-1157. *https://doi.org/10.5194/ejm-35-1149-2023*).

Tracking Thermally Induced Changes of Intermolecular Interactions in a Crystalline Hydrate, Forming Water Wire Within Self-Assembled Hydrophilic Nanochannels

Nanostructures formed by the self-assembly of modified or unmodified amino acids have significant potential for various biological and non-biological applications. In this context, γ-amino acids offer a wider conformational space due to their additional backbone torsional degrees of freedom and enhanced proteolytic stability compared to α-amino acids, warranting further exploration. Although modified single amino acid-based nanomaterials, such as nanobelts and hydrogels, have been developed using monosubstituted γ-amino acids derived from the backbone homologation of phenylalanine (Phe), there are no known examples of single γ-amino acid-based porous nanostructures capable of accommodating solvent molecules. Crystal structures of the modified γ4(R)Phe residue, Boc-γ4(R)Phe-OH, at different temperatures, revealed that hydrogen-bonded water molecules form a wire inside hydrophilic nanochannels. The dynamics of intermolecular interactions between the water wire and the channel's inner wall with changing temperatures were investigated through natural bonding orbital (NBO) calculations on single crystal structures obtained at various temperatures. The NBO results indicated that from 325K onward, the strength of water-water interactions within the water wire weakens, while water-inner wall interactions strengthen, suggesting a favorable reorientation of water molecules with increasing temperature. Prof. Simone Techert acknowledges the CMWS-Early Science Program of DESY/HGF. (K. Basuroy, J. de Jesus Velazquez-Garcia, S. Techert, Investigation of encapsulated water wire within self-assembled hydrophilic nanochannels, in a modified γ4-amino acid crystals: Tracking thermally induced changes of intermolecular interactions within a crystalline hydrate, Amino Acids 56 (2024) 9). *https://doi.org/10.1007/s00726-023-03372-4.*

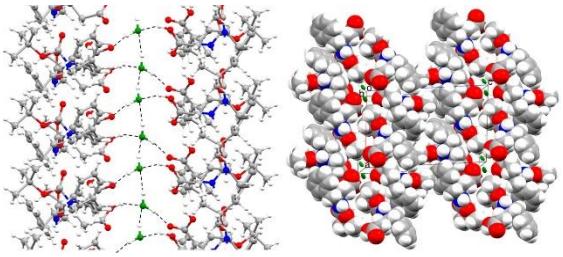
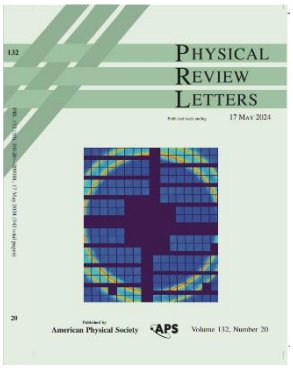


Figure Left: Packing of molecules in Boc-γ4(R)Phe-OH crystals at 80K showing the chain of water molecules in a hydrophilic channel, forming a zipper-like structure. Right: A space-fill model clearly shows how the water wire is contained within the nanochannel formed along the 21-screw axis.



Crystal Nucleation in Supercooled Atomic Liquids

The liquid-to-solid phase transition is a complex process that is difficult to investigate

experimentally with sufficient spatial and temporal resolution. A key aspect of the transition is the formation of a critical seed of the crystalline phase in a supercooled liquid, that is, a liquid in a metastable state below the melting temperature. This stochastic process is commonly described within the framework of classical nucleation theory, but accurate tests of the theory in atomic and molecular liquids are challenging. Here, we employ femtosecond x-ray diffraction from microscopic liquid jets to study crystal nucleation in supercooled liquids of the rare gases argon and krypton. Our results provide stringent limits to the validity of classical nucleation theory in atomic liquids, and offer the long-sought possibility of testing nonclassical extensions of the theory. This work was performed in a collaboration of CMWS researchers from GSI (Darmstadt), European XFEL (Schenefeld), DESY (Hamburg), and the Fritz-Haber-Institut (Berlin) within the framework of Pillar I. (J. Möller, A. Schottelius, M. Caresana, U. Boesenberg, C. Kim, F. Dallari, T.A. Ezquerra, J.M. Fernández, L. Gelisio, A. Glaesener, C. Goy, J. Hallmann, A. Kalinin, R.P. Kurta, D. Lapkin, F. Lehmkühler, F. Mambretti, M. Scholz, R. Shayduk, F. Trinter, I.A. Vartaniants, A. Zozulya, D.E. Galli, G. Grübel, A. Madsen, F. Caupin, R.E. Grisenti, Crystal Nucleation in Supercooled Atomic Liquids, Phys. Rev. Lett. 132 (2024) 206102). *https://doi.org/10.1103/PhysRevLett.132.206102.*

ANNOUNCEMENTS

Seminar series

Stay tuned for the next round of our biweekly seminars held on Thursdays at **12:00 via Zoom**. This coming winter semester taking place on: 24.10.24, 07.11.24, 21.11.24, 12.12.24, 09.01.25, 30.01.25.

CMWS Winter Semester 2024/25

(confirmed speakers)

24.10.24: Claudia Goy (DESY)
21.11.24: Axel Groß (University of Ulm)
12.12.24: Guilia Guibertoni (University of Amsterdam)

Save the date!

You are all cordially invited to our next CMWS Water Days 2025.

CMWS Water Days 2025

When: Feb 25th to Feb 27th, 2025
Where: DESY, CFEL I - III seminar rooms, building 99.
The link for registration will be distributed soon.
Registration will open in mid-December.
We kindly ask you to save the dates in your calendar.

Related workshops & conferences

American Geophysical Union Conference (AGU24)

This yearly conference is taking place this December 2024, in Washington, DC. Theme of this year is "What´s next for science". If you would like to know more about this conference please visit: *https://www.agu.org/annual-meeting.*

HBond 2025: 26th International Conference on Horizons in Hydrogen Bond Research

Hydrogen bonding plays a pivotal role in various fields such as biology, chemistry, astrophysics, and materials sciences. Scientists from diverse backgrounds convene at this conference to explore hydrogen bonding and other weak interactions using a wide array of experimental and theoretical approaches, covering all states of matter.

26th International Conference on Horizons in Hydrogen Bond Research

When: September 15th to 19th, 2025
Where: DESY, Hamburg

https://hbond2025.desy.de/

This conference will be held at DESY from Sep 15th to Sep 19th, 2025. We warmly invite all colleagues working on hydrogen bonding and related chemical interactions to join us at HBond2025 in Hamburg.

PEOPLE IN THE COMMUNITY

In this edition, we had the privilege of interviewing Emil Vogt from DESY and Vasily Artemov from EPFL School of Engineering. Discover their perspectives on science, molecular water, and life in the interviews below.

Emil Vogt

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

Emil: I began research with my PhD supervisor, Prof. Henrik G. Kjærgaard, at the University of Copenhagen during the second year of my BSc degree. Prof. Kjærgaard has spent much of his career studying the spectroscopy of water dimer and other important molecular complexes in Earth's atmosphere. His passion for this work was contagious, and I found it fascinating. Researchers have had, and still have, many challenges in understanding the thermodynamic and photophysical properties of weakly bound complexes. This was an immense surprise to me. With all the focus on macroscopic systems, how is it possible that our understanding of such important and small systems is so limited? As is often the case, the devil is in the details. One detail that makes water dimers complicated is the weak intermolecular hydrogen bond and the fact that each water molecule has two light hydrogen atoms. This combination of light atoms and weak interactions leads to highly delocalized vibrational states across its eight equivalent minimum energy configurations. Most of my research has focused, and largely still focuses, on describing the interaction of light with molecules that undergo large-amplitude motion.

Please tell us about your latest research project.

Emil: In the theory team of the Controlled Molecule Imaging group at CFEL, we are working on developing a new type of spectral approach. This approach transforms the challenging task of selecting coordinates and basis functions into an optimization problem. This helps to mitigate the persistent issue of the curse of dimensionality in nuclear motion problems and significantly improves spectral methods for systems with strong vibrational coupling and large-amplitude motion. Hopefully, you can read about it soon!

What was the most important advice someone gave you?

Emil: You learn from struggling, so learn to enjoy it. It is often comfortable to keep during what you are good at, but I do not think this is the best way to do science. Constantly challenging yourself by engaging in research slightly outside your field of expertise will enable you to draw connections that others have not considered before. It also helps you interact with and understand researchers, which contributes to your growth as a scientist.

When do you have your best ideas?

Emil: Bike ride after a tough game of squash. This clears my mind and frees me from the details of my work. I have always found that stepping back after being fully emerged in a subject enables creative thinking.

How do you balance your professional and personal life?

Emil: I try my best to spend as much time as possible with my girlfriend and our dog, as well as play squash roughly three times a week. I have always

enjoyed sports, and there is no better way to clear your mind than to push your heartrate and lungs to the limit.

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

Emil: Read the literature. I think the publication pressure really gets to especially PhD students today, and it is easy to spend all your energy and time on the details of your work. My advice is to force yourself to spend somewhere between six and eight hours a week on reading (and taking notes). This is not added time to your work week, but a part of it. Make a good cup of coffee, slow down, and read about topics that interest you! This should not be only the papers that your supervisor and colleges are interest in.

Vasily Artemov

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

Vasily: During my masters, I tackled the challenging problem of isolating ortho- and para-spin isomers of water, which had been predicted decades earlier but had not yet been separated. These isomers naturally exist in a 3 to 1 ratio and differ in their net nuclear spin 1 for ortho and 0 for para water. Together with my colleagues, I developed a selective real-time spectrometer of the ortho-para composition of water and obtained ortho-enriched samples. However, the enriched samples have been recombining to equilibrium for less than a microsecond, contradicting the prevailing model of water of that time.

This contradiction sparked my deep interest in the molecular structure of water. For the next ten years, first as a Ph.D. student and later as a head of the laboratory of intermolecular interactions spectroscopy, I spent studying atomic-molecular dynamics in water. This work led me to an original model, which I called the ionic model of water. The key findings from this journey are detailed in the monograph, The Electrodynamics of Water and Ice.

Please tell us about your latest research project.

Vasily: My current interest is in sustainable energy storage. You probably heard about Nikola Tesla who was exploring deriving electricity from the global water cycle. Just imagine that one lightning releases gigawatts of electricity stored in the atmospheric water. Nevertheless, for storage purposes, we have traditionally relied on complex, often rare, elements for electricity storage. Unlike Nikola's, my current research focuses on developing new sustainable technologies for energy harvesting, conversion, and storage using laboratory-made natural aqueous interfaces. These technologies aim not only to mitigate but also benefit from inevitable global climate change.

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

Vasily: There are many open questions in the field. For example, the exact role of water in the biological systems' metabolism remains elusive. Water's molecular structure plays a crucial part in biopore signaling, DNA translocation, protein aggregation, and the transmission of nerve impulses. However, we still lack a detailed understanding of the underlying mechanisms. Another area where the properties of water are of significance is ionotronics. Current models of aqueous electrolytes are inadequate in scenarios of sub-nanometer confinement. It's time to move beyond the traditional models and explore new dynamic models of aqueous electrolytes to unlock potential technologies such as power generation and storage, cost-effective water desalination, and bio-mimicking computing.

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?

Vasily: I am looking for open-minded people, both young and adult, not afraid of testing unconventional original ideas and converting

fundamentals into sustainable technologies of the future. Fast spectroscopic techniques, X-ray spectroscopy, XFEL, and neutron scattering experiments are of particular interest.

What was the most important advice someone gave you?

Vasily: I didn't receive much advice, so books have primarily shaped my mindset. Recently, while learning French, I reread Le Petit Prince and was struck by the quote: "L'essentiel est invisible pour les yeux"—"What is essential is invisible to the eye." I think it's good advice, although perhaps not entirely relevant for those working in optics research.

When do you have your best ideas?

Vasily: My ideas come in different circumstances. There is no correlation between place, time, and ideas. They seem to exist on orthogonal planes.

What does make you laugh?

My family and my dog. We have a lot of fun together.

How do you balance your professional and personal life?

Vasily: Being part of a scientific family blurs the distinction between professional and personal life; everything naturally finds its balance. If I am not in the office on weekends, I enjoy playing guitar, swimming several kilometers in the lake, hiking, and traveling.

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

Vasily: That's a good question... I like art and we are traveling around the world to meet favorite painters' masterpieces. I like Bruegel. Can spend hours in front of his canvases.

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

Vasily: I would refrain from advising since each research track is unique and cannot be repeated. As Plato noticed, "Nothing exists, but everything becomes." Just follow your dreams.

CONFERENCES & WORKSHOPS OVERVIEW

2024

American Geophysical Union Conference (AGU24)
December 9th -13th, 2024. Washington, DC, USA.
https://www.agu.org/annual-meeting

2025

COMING SOON:

CMWS Water Days 2025
February 25th-27th, 2025. Hamburg, Germany

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