

CMWS WATER DAYS 2025

Location, if not indicated differently: FLASH seminar room, building 28c, 2nd floor, DESY

Programme

Tuesday February 25

13:00 Registration

Welcome and General CMWS Session

Chair: Claudia Goy (DESY)

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|-------|-----------------------------------|--|
| 13:30 | Franz Kärtner (DESY / UHH) | Welcome to DESY and Photon Science |
| 13:50 | Melanie Schnell (DESY / CAU Kiel) | Status & future of CMWS |
| 14:10 | Traugott Scheytt (TU BA Freiberg) | How molecular water research benefits from facilities and living labs at TUBAF |
| 14:25 | Ellen Adams (HZDR) | Molecular water science at Helmholtz-Zentrum Dresden-Rossendorf |
| 14:40 | Coffee break | |

Science Session 1

Chair: Patrick Huber (DESY/ TUHH)

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| 15:10 | Olivier Vincent (CNRS / U Lyon 1) | Humidity-triggered phase change and transport of water and solutions in nanopores |
| 15:50 | Volkan Filiz | Membranes and Synchrotron |
| 16:10 | Max Rauscher (MU Loeben) | Flow-dependent capacitive water deionization: A time- and position-resolved synchrotron investigation |
| 16:30 | Randeer Pratap Gautam (DESY / U Siegen) | Investigation of protein diffusion in ferritin systems at low temperatures using XPCS |
| 16:50 | Estelle Becquevort (KU Leuven / DESY) | In situ NMR/dielectric spectroscopy unravelling water – ice dynamics in nanoconfined clathrate formation |

17:30 Lab tours

18:30 Poster Session & Dinner (Canteen extension, building 9a, 1st floor)

Wednesday February 26

Science Session 2

Chair: Iain Wilkinson (HZB)

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| 08:50 | Petr Slavicek (U Chemistry and Technology, Prague) | Electrons in water: birth, transport and reactivity |
| 09:30 | Anthony Ferté (DESY) | Electron impact excitation and ionization of liquid water |
| 09:50 | Nicolas Velasquez (FHI) | Ultrafast charge transfer in aqueous L-cysteine |
| 10:10 | Svenja Hövelmann (DESY / CAU Kiel) | X-ray scattering studies of light induced dynamics at liquid interfaces and biological membranes. |
| 10:30 | Coffee break | |

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| 11: 00 Career Workshop (FLASH seminar room, building 28c, 2 nd floor) | Dedicated to students, Postdocs and young researchers Max 20 participants - Interest to participate should be indicated during registration |
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12:30 Festive Signature of Declaration & Reception (CFEL foyer, building 99)

CMWS Inauguration Symposium (CFEL I-III, building 99)

Chair: B. Redlich (DESY)

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| 14:00 | Welcome notes | |
| 14:45 | Patrick Huber (DESY/ TUHH) | BlueMat: A research initiative on water-driven materials |
| 15:05 | Sakura Pascarelli (EuXFEL) | Molecular water research at European XFEL |
| 15:25 | Sören Jaspers (Beiersdorf AG) | Water and skin |
| 15:45 | Nönne Prisle (DESY/ UHH) | Keynote lecture: Water and aerosols: molecular interactions with impacts from personal to global |
| 16:15 | Closing remarks | |
| 16:30 | Coffee break | |

Science Session 3

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| | | <i>Chair: Simone Techert (DESY/ U Göttingen)</i> |
| 17:00 | Donatella Loru (DESY) | Microsolvation of Polycyclic Aromatic Hydrocarbons in Water: Insights from Rotational Spectroscopy |
| 17:40 | Avinash Chettri (U Potsdam) | 2D-IR Spectroscopy reveals structural heterogeneity in GLFG-rich hydrogels as models for the nuclear pore complex |
| 18:00 | Juliette Leroux (UHH) | Influence of a single water molecule on the X-ray absorption spectra of gas-phase phosphotyrosine |

19:00 Public evening lecture in german language

(DESY Auditorium, building 5)

Robin Santra (DESY, CFEL)

"Die schnellsten molekularen Prozesse in Wasser"



Thursday February 27

Science Session 4

Chair: Jack Lin (U Oulu)

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| 08:50 | Sven Schroeder (U Leeds) | Precipitation and dissolution of solids in water: Kinetics beyond classical nucleation theory |
| 09:30 | Llorenc Cremonesi (U Milan) | Experimental multiparametric characterisation of aerosols through light scattering |
| 09:50 | Melanie Schnell (DESY/CAU) | A tiny droplet of acid: Hyperfine-resolved rotational spectroscopy reveals HCl dissociation upon microsolvation |
| 10:10 | Markus Osterhoff (U Göttingen) | Taming the bubbles: Cavitation dynamics revealed by XFEL pulses |

10:30 Coffee break

Science Session 5

Chair: Sergio Speziale (GFZ)

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| 11:00 | Rachel Husband (DESY) | Phase transition kinetics in superionic ice |
| 11:40 | Divyanshu Ranjan (DESY/ U Rostock) | Probing ice giants Interiors with shock compression |
| 12:00 | Katrin Amann-Winkel (U Mainz) | Intrinsic dynamics in amorphous ices measured by XPCS |
| 12:20 | Kyung Hwan Kim (POSTECH, Korea) | Experimental studies of the liquid-liquid critical point and fragile-to-strong transition of liquid water using FELs |
| 12:40 | Matthias Sperl (DLR) | Glassy dynamics of water |

14:00-16:00 Pillar Meetings

(Individual meeting rooms: FLASH, SR in Bld 94/3rd floor, CFEL IV, CFEL I, CFEL II, CFEL III)

Pillar 1

Pillar 2

Pillar 3

Pillar 4

Pillar 5

18:30 Poster Session & Dinner
 (Tuesday 25th, Canteen extension, building 9a, 1st floor)

| Author(s) | Affiliation | Title |
|----------------------------------|---|--|
| Abhirami Udayabanu | Physics of life Cluster of Excellence, TU DRESDEN | TBA |
| Artur Czajkowski | Physics of Life Cluster of Excellence, Technische Universität Dresden | Protein modifications and ionic strength show the difference between protein-mediated and solvent-mediated regulation of biomolecular condensation |
| Camilo Jose Zapata Segura | Physics of Life Cluster of Excellence, TU Dresden | TBA |
| Chen Shen | Deutsches Elektronen-Synchrotron DESY | Single-shot reflectivity acquisition from liquid surfaces by GISAXS |
| Dana Bloß | | Intermolecular processes in core-hole decay of microsolvated organic molecules |
| Denis Tikhonov | CFEL-DESY | Simulating strong-field-induced and X-ray-probed dynamics of saline water |
| Florian Trinter | Fritz-Haber-Institut Berlin | Radiationless decay spectrum of O 1s double core holes in liquid water |
| Iason Andronis | Stockholm University | Supercritical density fluctuations and structural heterogeneity in supercooled water-glycerol microdroplets |
| Isabell Erdmann & Klara Holl | Johannes Gutenberg-Universität | Aqueous solutions under extreme conditions |
| Joana Valerio | European XFEL | Liquid sample delivery at European XFEL - new developments |
| Katinka Horn | ETH Zürich | RABBITT on large water clusters |
| Likhitha Chakra Priya Pulibandla | | Exploring the thermodynamics of fus and its interactions with ATP |
| Lisa Nucke | Helmholtz-Zentrum Dresden-Rossendorf | Influence of different membrane mimetic systems on intra-membrane protein hydration and function |
| Louisa Kraft | Max Planck Institute for Polymer Research | Three-phase contact line dynamics on moving fibers measured by X-ray holography |
| Markus Osterhoff | Röntgenphysik, Uni Göttingen | Taming the bubbles: Cavitation dynamics revealed by XFEL pulses |
| Martin Andersson | King Fahd University of Petroleum and Minerals | The shape of water – how cluster formation provides a unifying explanation of water's anomalous properties and the hydrophobic effect |
| Nathaniel Okpara | DESY-CFEL Theory Group | Computational modelling of electron solvation in liquid water |
| Nele Striker | DESY | Phase behavior of aqueous silica-PNIPAm dispersions under high hydrostatic pressure |
| Niels Gießelmann | Johannes Gutenberg-Universität Mainz / MPI für Polymerforschung | The structure of water and ice under confinement in mesoporous organosilicas |
| Rahim Ullah | Deutsches Elektronen Synchrotron DESY | Liquid Flat-jet for ultrafast spectroscopy of molecules in aqueous solution at FELs |
| Robert Farla | FS-PETRA-D (FS-PET-D Fachgruppe P61 (Wiggler BI.)) | The role of H ₂ O at high pressures in the LVP at P61B |

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| Shaoheng Wang | University of Hamburg | Water vapor sorption of the salt particles in nanopores |
| Siddhanth Shishodia | Max planck institute of polymer research | TBA |
| Tobias Eklund & Siddhanth Shishodia | Johannes Gutenberg Universität Mainz | Optical and X-ray studies on amorphous solid water |
| Wagner Ribeiro da Silva Neto | ISRR-Bessy II/HZB | Direct observation of symmetry breaking in the 3MLCT state of the N3 dye in water by X-Ray absorption spectroscopy |
| Yizhi Liu | Max Planck Institute for Polymer Research | Numerical simulation of heat transfer in nanoscale amorphous water |
| Yusaku Terao | University of Kassel | Multielectron spectroscopy of solvated iodide anion |