



Centre for Molecular Water Science (CMWS)

Melanie Schnell

2nd Helmholtz-CAS Workshop

More information:
www.cmws-hamburg.de

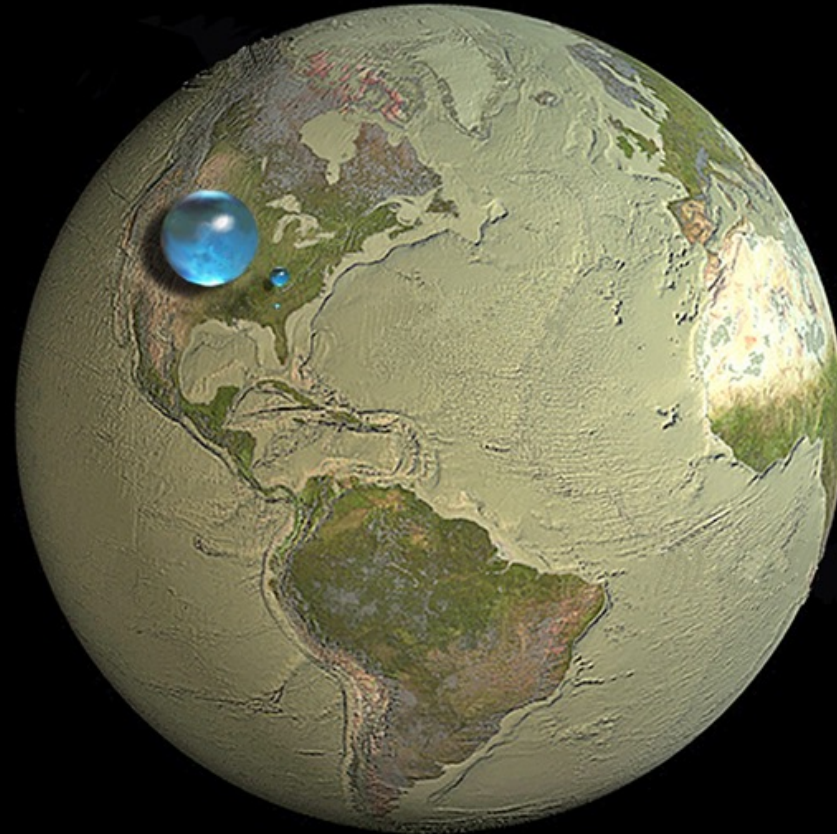
HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

CMWS
Centre for Molecular
Water Science

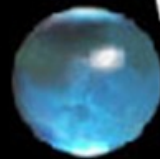


All Water on Earth

sphere of
about 1385
km in
diameter



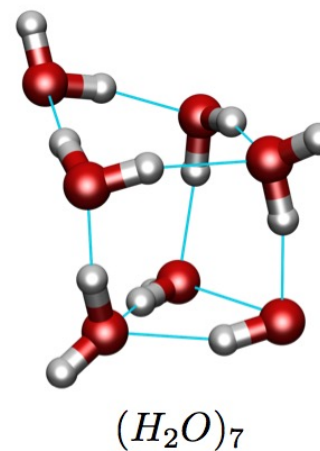
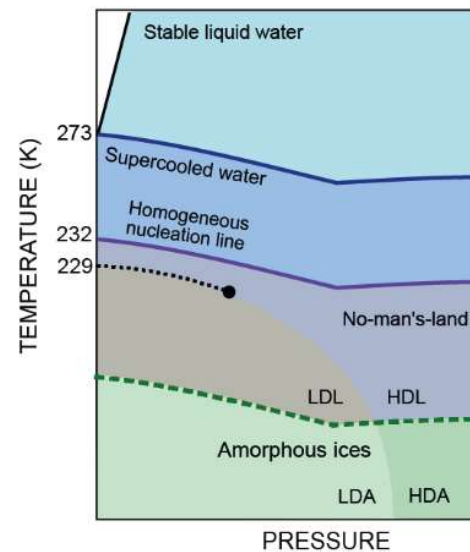
Water in, on, and above the Earth



- Liquid fresh water
- Freshwater lakes and rivers

Howard Perlman, USGS
Jack Cook, Adam Nieman
Data: Igor Shiklomanov, 1993

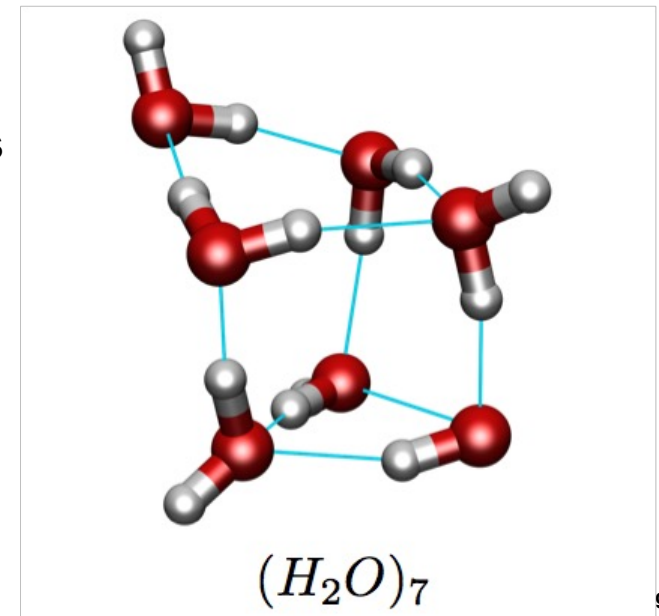
The anomalies of water



The situation

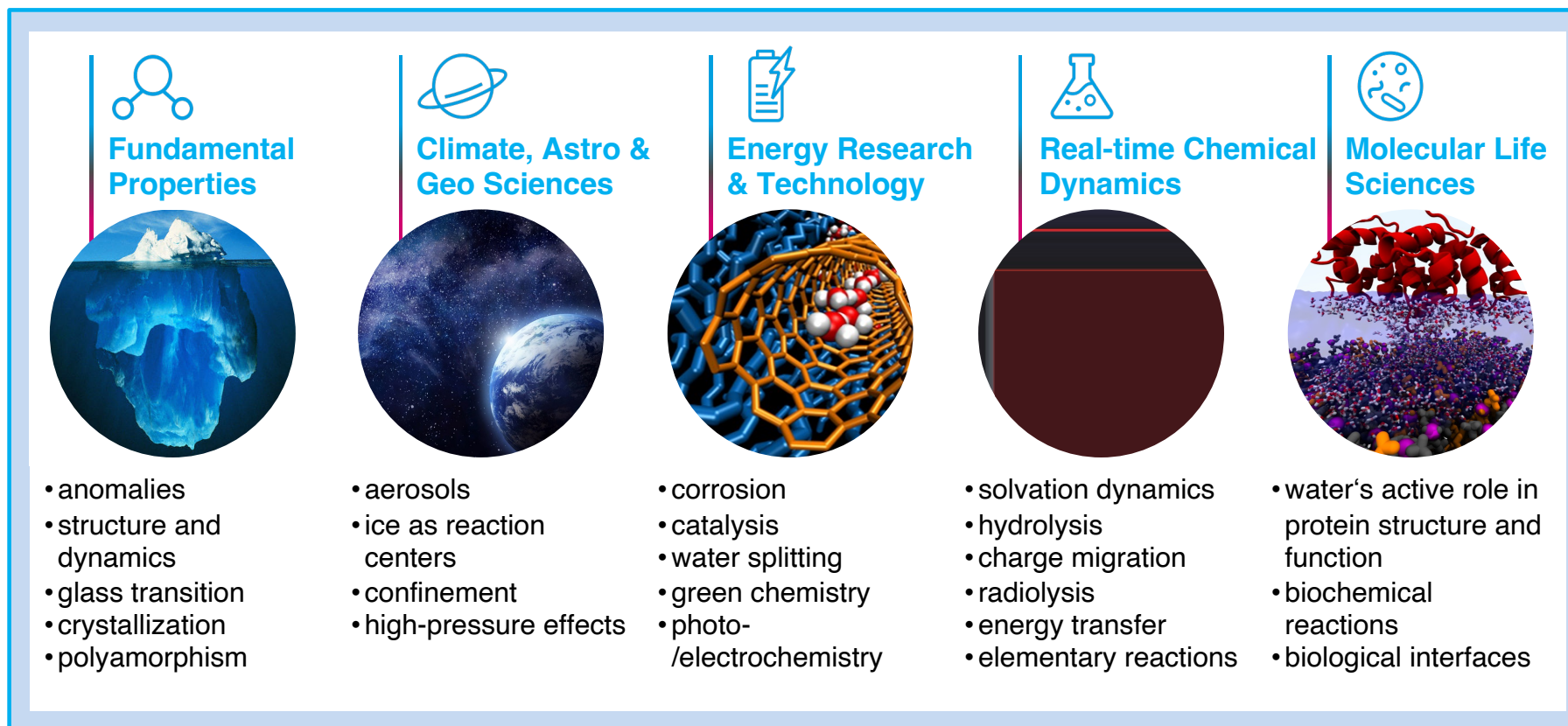
- Water matters (energy, agriculture, life)
- Water is a rare resource
- Water is probably the most anomalous liquid that we know, with many fundamental properties still to be understood
- Water is the solvent of life, also made possible by its characteristic hydrogen bonding
- Water is highly relevant for infection research – e.g. aerosols

**Forge an international cooperation to enable
A MOLECULAR UNDERSTANDING OF WATER and its role in
different applications**



Five research pillars

More than 60 international partners

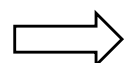
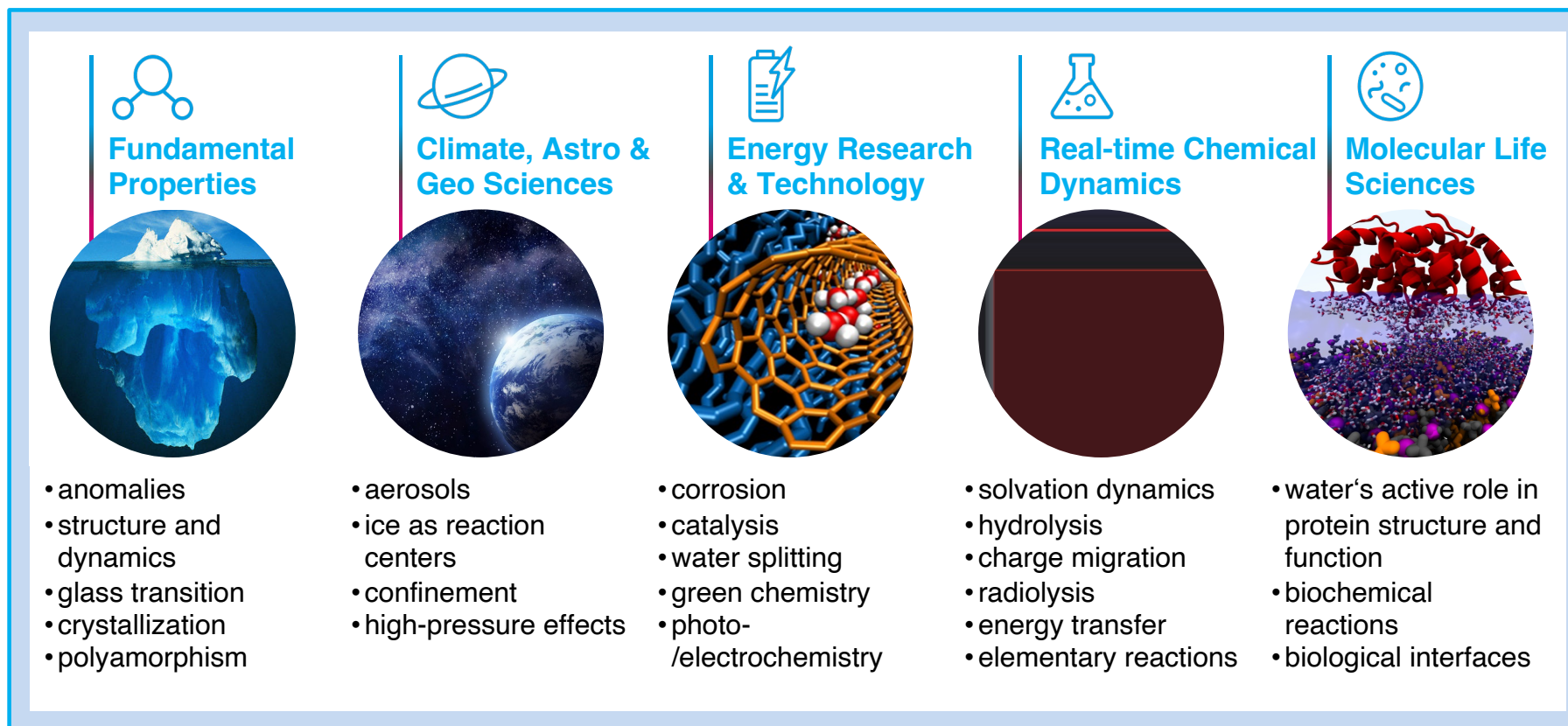


⇒ Each pillar is represented by speakers; regular meetings

⇒ Annual CMWS Water days at DESY

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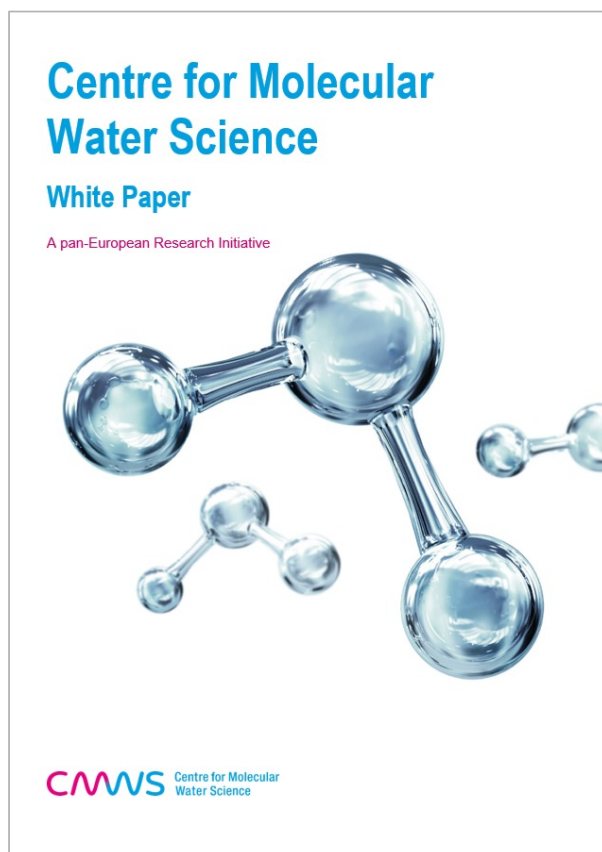


Important science cases for the Hamburg photon sources

CMWS White & Strategy Paper

The White Paper

Motivation, research agenda, and vision of the CMWS



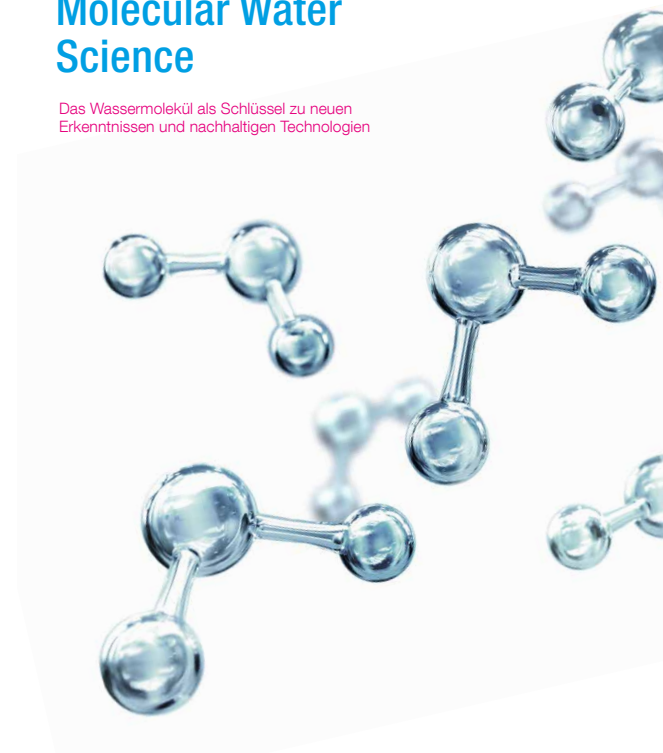
**114 researchers from
45 institutions (more
than 15 countries)
covering 5 research
pillars**

To be downloaded from
www.cmws-hamburg.de

The Strategy Paper

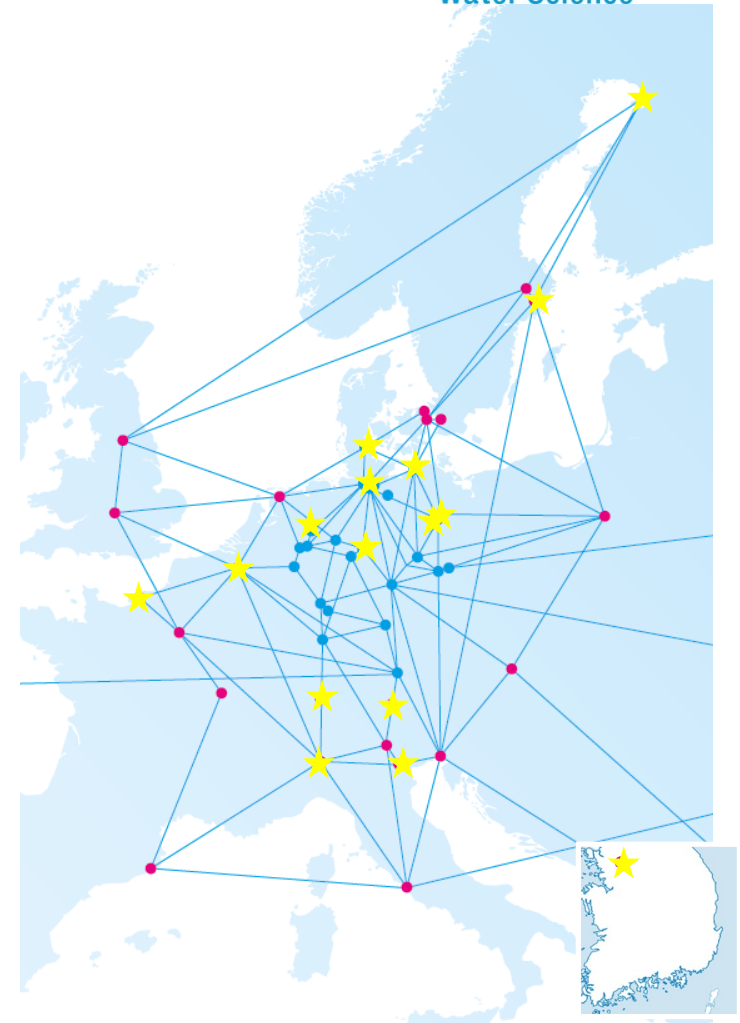
**Centre for
Molecular Water
Science**

Das Wassermolekül als Schlüssel zu neuen
Erkenntnissen und nachhaltigen Technologien



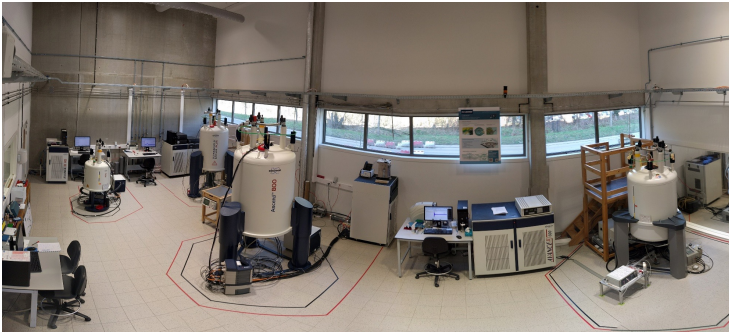
Science Program with joint PhD students

- **30 joint projects for PhD students** (from 3 calls)
- Covering all **5 research areas**
- Joint projects funded on a 1:1 basis by DESY and CMWS partner:
 - Dedicated focus on the research challenges outlined in the White Paper
- Currently: Working out funding schemes to develop it into a **regular science program** with joint, interdisciplinary projects



Hub structure

More than 60 international partners



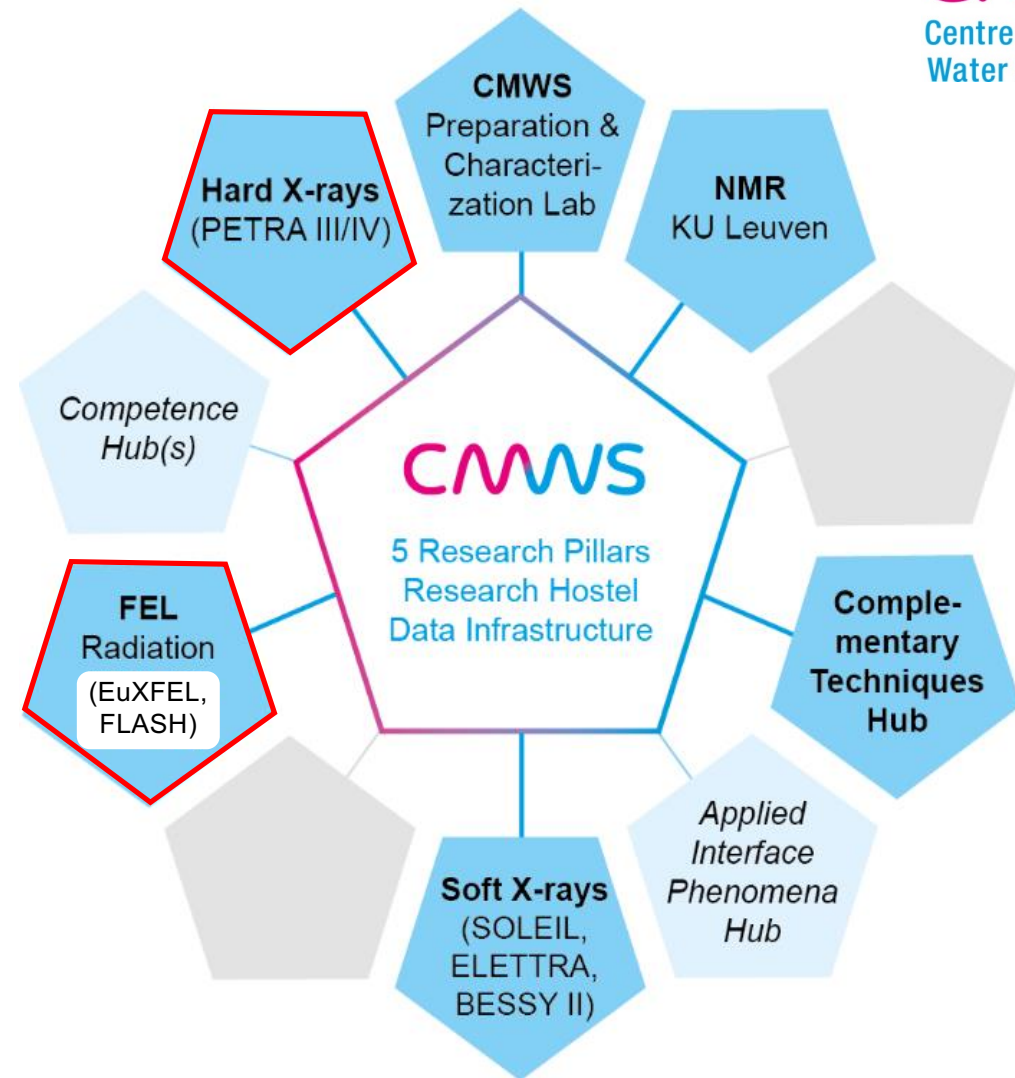
1st CMWS HUB:
High Field NMR (NMRCoRe @ KU Leuven, Belgium)



2 CMWS Laboratories @ DESY

EQUIPMENT:

- Raman spectrometer
- Multi-user FTIR spectrometer
- Ion-mobility spectrometer
- Water-cluster-dynamics endstation

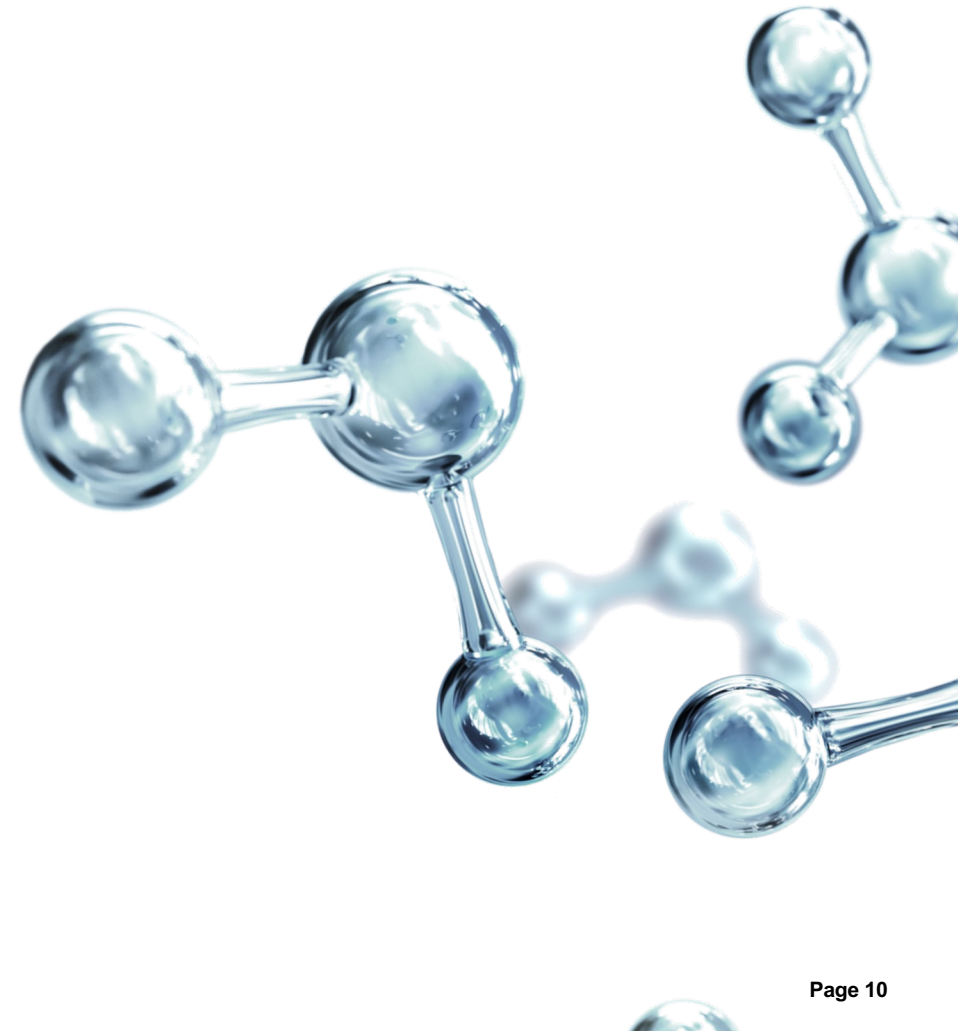


Targeted Calls

- European XFEL targeted call on *Molecular Water Science*
 - 30 Expressions of Interest received
 - 25 spokespeople invited to submit full proposal
 - 8 selected

- PETRA III call for Targeted Challenge-driven Proposals on *Molecular Water Science*
 - collaborations of at least three independent research groups
 - request beamtime at several different experiments and beamlines
 - has to comprise three or more subprojects

 - 6 proposals received
 - 1 selected

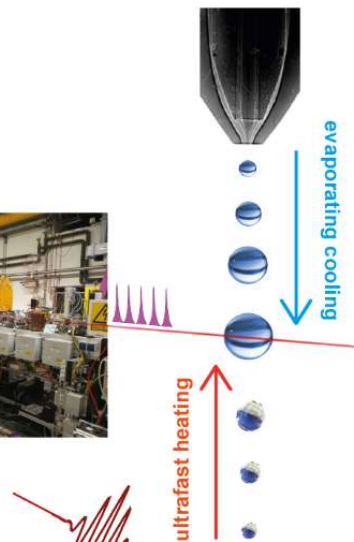


Schematic illustration of an X-ray experiment in "No man's land"

- Requires sophisticated sample delivery & manipulation
- Advanced X-ray technologies (e.g. detectors)

Gas dynamic virtual nozzle:
Pure liquid water accelerated and compressed by a stream of nitrogen at high pressure μm droplets at 0.1 sound velocity are produced

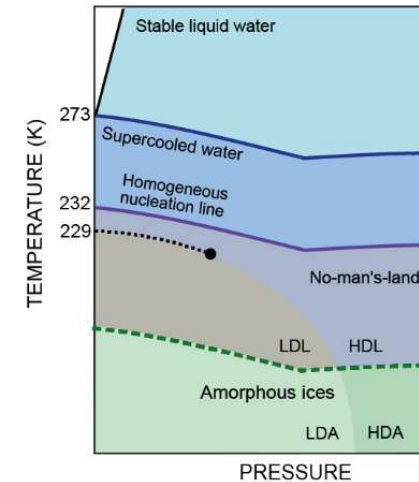
European XFEL:
3.4 km tunnel length, superconducting accelerators boost the electrons up to 17.5 GeV, pulses of hard Xrays ~ 50 fs long generated in the MHz range.



Ultrafast pump laser:
Pulse length between 100 – 10 fs, wavelength of 800 nm, and power up to 3 mJ per pulse



amorphous ice



AGIPD detector:
1 Megapixel detector, up to 352 scattering images at 6.5 MHz (one image every 154 ns)

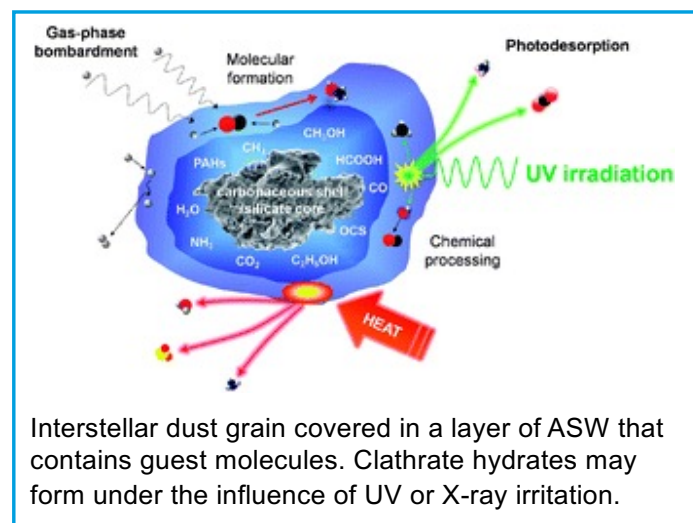
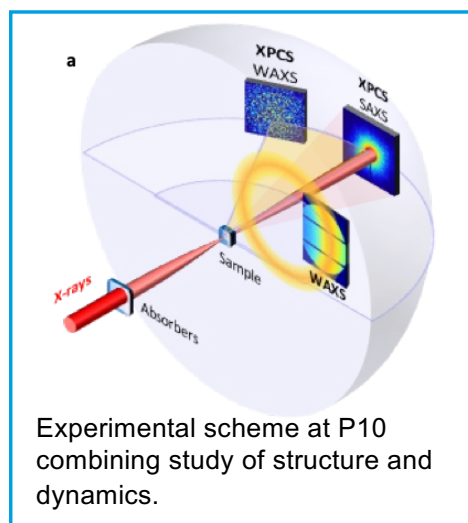
Targeted challenge-driven proposal call at PETRA III on water

From Amorphous Ices to Clathrate Hydrates

- Principal Investigators
 - Katrin Amann-Winkel (MPI Mainz)
 - Felix Lehmkuhler (DESY)
 - Thomas Loerting (U Innsbruck)
- Beamtime for 2023/2024
 - 54 shifts (3 weeks) P10
 - 36 shifts (2 weeks) at P21.2

Understand dynamics and kinetics of phase transitions in amorphous ices

- Dynamics near the glass transition of different amorphous ices (e.g. HDA, HGW) **[P10]**
- Pore collapse and clathrate hydrate formation from guest-loaded ASW **[P10]**
- Real-time kinetics of hydrate formation **[P21.2]**



Networking and outreach

- Annual “CMWS Water Days”
- Young researchers’ meeting (newly installed at the Water Days 2023)
- Bi-weekly CMWS lunch seminar (online) of the international network of the CMWS, started summer 2021 (23 events so far)
- PIER workshop on joint DESY/UHH research perspectives in molecular water research (June 2022)
- Several outreach activities and media coverage: “Physik in unserer Zeit”, “Physik Journal”, “FAZ Sonntagszeitung”, “Bild der Wissenschaft”, “Bunsenmagazin”, Helmholtz resonator podcast ...



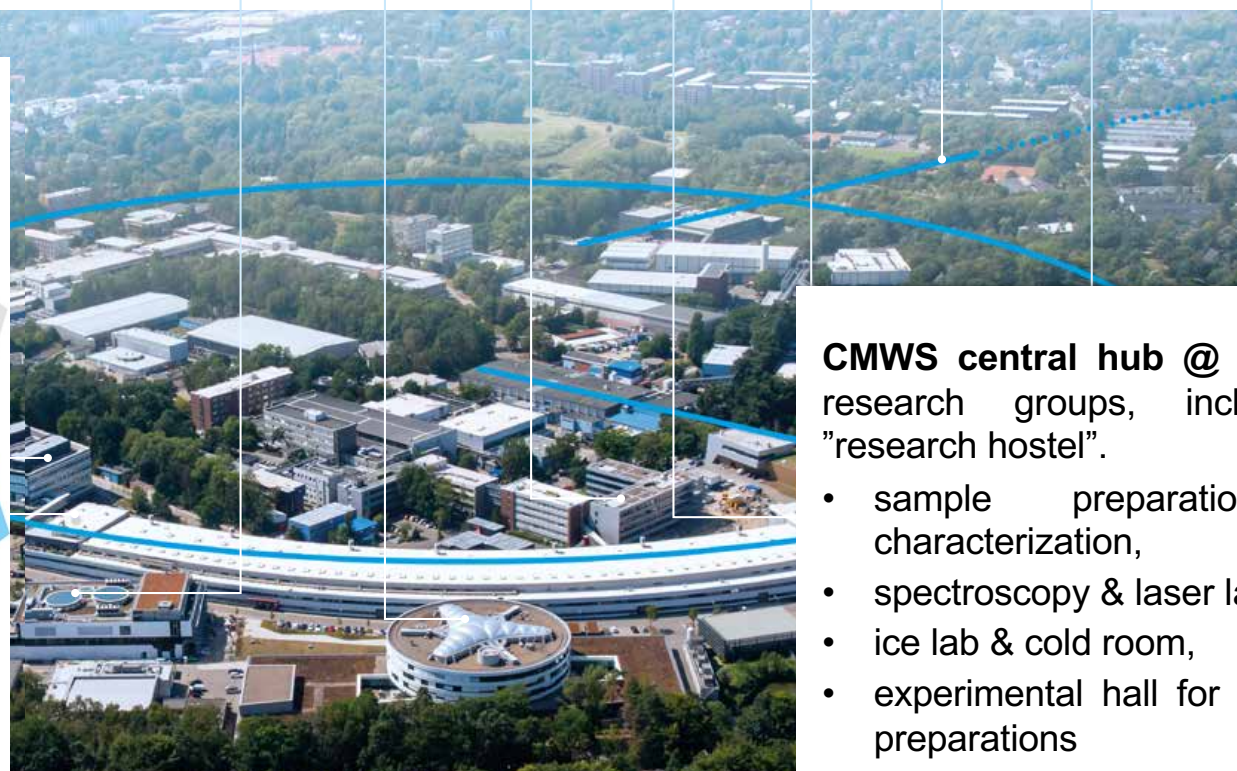
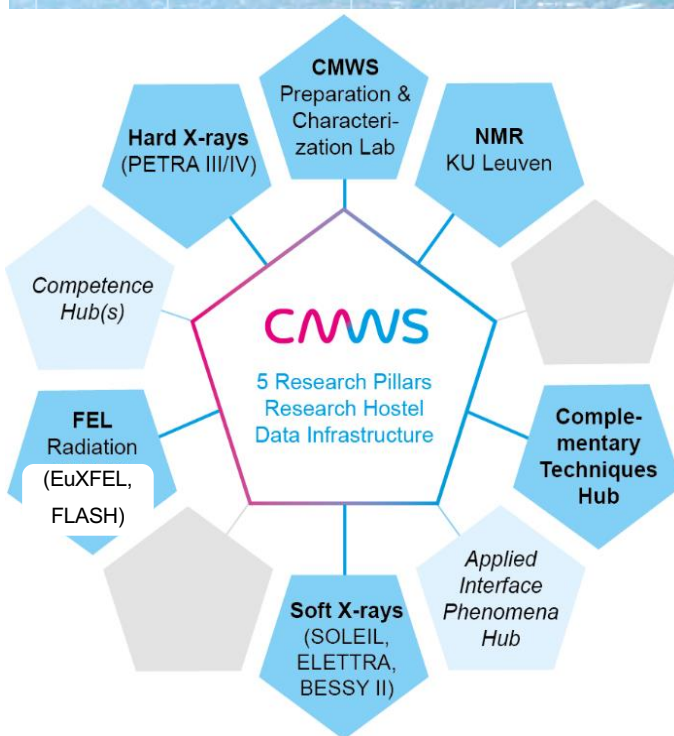
Strategic NEXT steps

- **Consortium declaration**
- **Development of a funding strategy**
 - Application for a CMWS central hub at DESY via the Helmholtz strategic investment program (application summer 2024)
 - To strengthen and extend the CMWS science program via proposals of individual consortia (German Science Foundation, German Federal Ministry of Education and Research, clusters of excellence, EU doctoral networks).



A home for the CMWS – the Hamburg central hub

ChyN Center for Hybrid Nano-structures
HARBOR Hamburg Advanced Research Centre for Bioorganic Chemistry
EMBL European Molecular Biology Laboratory
CSSB Centre for Structural Systems Biology
CMWS Centre for Molecular Water Science
MPSD Max-Planck-Institut für Struktur und Dynamik der Materie
CFEL Center for Free-Electron Laser Science
CXNS Centre for X-ray and Nano Science
PETRA III/IV Positron-Elektron-Tandem-Ring-Anlage
FLASH Freie-Elektronen-Laser in Hamburg
European XFEL European X-Ray Free-Electron Laser
Start-up Labs Bahrenfeld



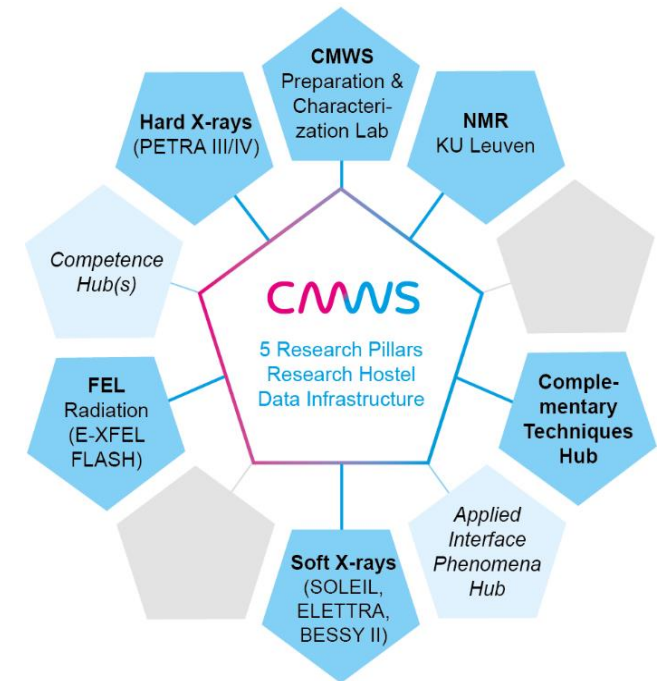
CMWS central hub @ DESY for research groups, including a "research hostel".

- sample preparation and characterization,
- spectroscopy & laser labs,
- ice lab & cold room,
- experimental hall for beamtime preparations

The situation

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- **Water is a rare resource**
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Thank you!