

Molecular Water Science

23 January 2024 / XHQ, Room E1.173, European XFEL

This workshop shall prepare the second call for User Experiments on Molecular Water Science to be opened for the allocation period 2025-I. The program will present an overview on open questions and ongoing activities in the field by international experts, report on the outcome of the first call and bring together interested users for the second call to share information, discuss joint research projects and form collaborations.

Organiser: Sakura Pascarelli, Gerhard Grübel

Contact: Gerhard.gruebel@xfel.eu

Tuesday, 23rd January 2024 (Preliminary agenda)

Time	Session	Speaker	Facility
9:00-9:30	Welcome & Introduction	S. Pascarelli / G. Gruebel	European XFEL
9:30-10:00	Computational Exploration of Supercooled Water	P. Debenedetti	Princeton University
10:00-10:30	Recent computational studies of the liquid-liquid transition in supercooled water	F. Sciortino	University of Rome
10:30-11:00	Hidden crystallization pathways of supercompressed H ₂ O at room temperature	G. W. Lee	KRISS
11:00-11:30	Coffee break		
11:30-12:00	Ice structure and formation of crystalline order during the freezing of supercooled water drops	C. Stan	Rutgers University
12:00-12:30	Crystallization kinetics studied by single-shot and single-particle X-ray diffraction	A. Niozu	Hiroshima University
12:30-13:00	Organization of water and ions at the surface of electrolyte solutions	M. Bonn	MPI for Polymer Research
13:00-14:30	Lunch break + facility tour		
14:30-15:00	The CMWS - a strategic approach to reveal the peculiar properties of water	M. Schnell	DESY
15:00-15:20	TopCall I	J. Sellberg	KTH Royal Institute of Technology Stockholm
15:20-15:40	Ultrafast X-ray solution scattering reveals "breathing" dynamics of a broken tetrahedral cage	Q. Kong	SOLEIL
15:40-16:00	Ultrafast dynamics and structure formation in supercooled aqueous systems	F. Lehmkuhler	DESY
16:00-16:30	Coffee break		
16:30-16:50	Atmospheric aerosols - open questions and how XFELs might help	N. Prisle	University of Oulu
16:50-17:10	Molecular Water Science as a Game-Changer: Paving the Way for Sustainable Energy Solutions	E. Breynaert	KU Leuven
17:10-17:30	Bio	H. Müller-Werkmeister	University of Potsdam



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17:30-18:30	Discussion (15') Write a good proposal (15')	A. Madsen	European XFEL
18:30-20:00	Dinner - Beamstop		
20:00-21:30	Matchmaking Discussion		