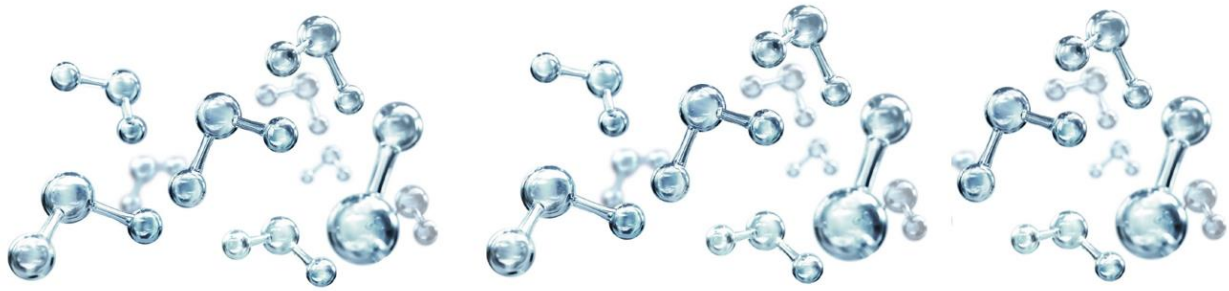
Summer Semester 2021

CMWS Centre for Molecular Water Science



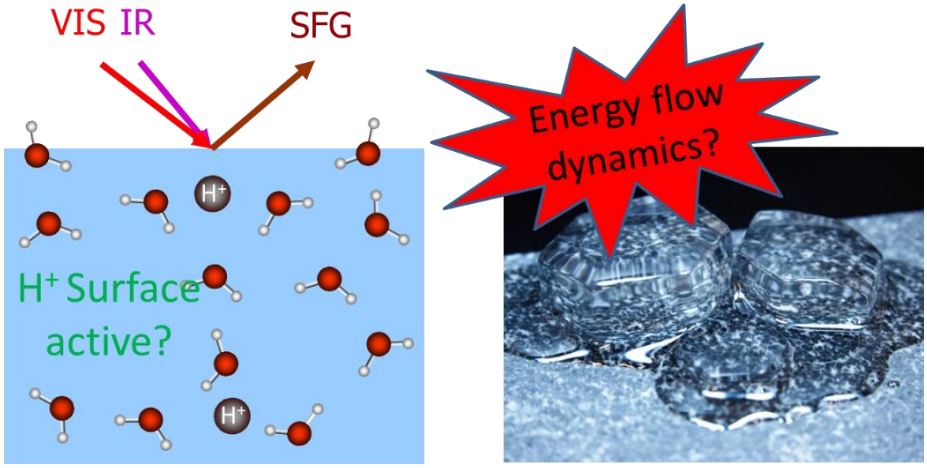
8th of July 2021
12:00 h

Ellen Backus

Institut für Physikalische Chemie, Universität Wien Max-Planck-Institut für Polymerforschung, Mainz

The surface of ice, liquid water, and acidic water

The structure and dynamics of interfacial phenomena is not only interesting from a fundamental point of view, but also relevant for many atmospheric, geochemical, and electrocatalytic processes. In the first part of the talk, we will look into the behaviour of hydroxide and hydrated protons, the auto-ionization products of water. By using the surface-sensitive vibrational sum frequency generation spectroscopy – basically providing the vibrational spectrum of just the interfacial layer – on the O-H stretch region, the onset concentration of surface adsorption at the water-air surface of hydrated protons and hydroxide ions can be determined. As such the relative surface-activity has been obtained [1]. Moreover, changes in the spectral signature of the so-called free OH molecule sticking out in the air are used to determine the adsorption free energy of the proton [2]. In the second part of the talk we will look into vibrational energy dynamics on the surface of ice, potentially important for atmospheric chemistry where reactions are taking place on the ice surface. A comparison to liquid water surfaces, reveals accelerated vibrational energy relaxation and dissipation at the ice sur- face for hydrogen-bonded OH groups. In contrast, free-OH groups sticking into the vapor phase exhibit substantially slower vibrational dynamics on ice [3]. The results will be related to the structural differences between ice and water and to the high catalytic activities of ice.



References

[1] S. Das, M. Bonn, E.H.G. Backus, Angew. Chem. Int. Ed. 58 (2019) 15636
[2] S. Das, S. Imoto, S. Sun, Y. Nagata, E.H.G. Backus, M. Bonn, J. Am. Chem. Soc. 142 (2020) 945
[3] P. Sudera, J.D. Cyran, M. Deiseroth, E.H.G. Backus, M. Bonn, J. Am. Chem. Soc. 142 (2020) 12005

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24th of June 2021
12:00 h

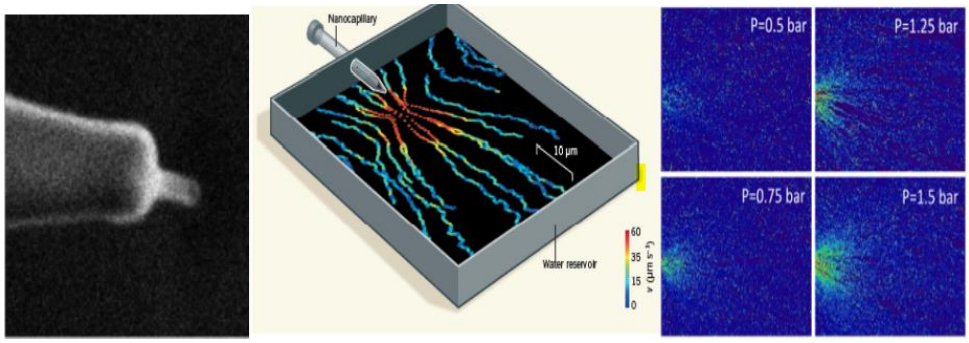
Lydéric Bocquet

Micromégas team, Laboratoire de Physique Ecole Normale Supérieure and CNRS, Paris

Scale oddity of water transport in nanochannels

In this talk, I will discuss various experimental and theoretical results that we obtained recently in our team on the transport of water and ions in ultra-confinement. I will in particular focus on the odd properties of the water-carbon couple, which highlights a variety of exotic transport properties that we will discuss and rationalize, such as ultra-low friction [1,2], specific charge adsorption, strongly non-linear transport and mechanosensitivity [3,4], …

I will show how these specificities can be used as building blocks to build a ionic machinery, from ion pumps to artificial neuromorphic behavior [5] and the development of elementary ion-based computing.



References

[1] “Massive radius-dependent flow slippage in single carbon nanotubes”, E. Secchi, S. Marbach, A. Niguès, D. Stein, A. Siria and L. Bocquet, Nature 537 210 (2016).
[2] “Fluctuation-induced quantum friction in nanoscale water flows”, N. Kavokine, A. Robert, M.-L. Bocquet and L. Bocquet, submitted (2021).
[3] “Molecular streaming and voltage-gated response in Angström scale channels”, T. Mouterde, A. Keerthi, A. Poggioli, S. Dar, A. Siria, A.K. Geim, L Bocquet and R. Boya, Nature 567 87 (2019).
[4] “Mechanically activated ionic transport across single digit carbon nanotubes”, A. Marcotte, T. Mouterde, A. Nigues, A. Siria and L. Bocquet, Nature Materials 19 1057 (2020). [5] “Principles of Hodgkin-Huxley iontronics with two-dimensional nanofluidic memristors”, P. Robin, N. Kavokine, and L. Bocquet, to be published in Science (2021).
[5] “Principles ofHodgkin-Huxley iontronics with two-dimensional nanofluidic memristors”, P. Robin, N. Kavokine, and L. Bocquet, to be published in Science (2021).

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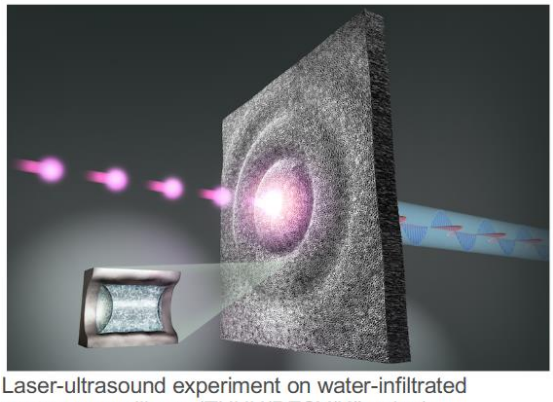
10th of June 2021
12:00h

Patrick Huber

Hamburg University of Technology and Deutsches Elektronen-Synchrotron DESY

Water confined in nanopores: What do we know about it and what is it good for?

Water confined in pores a few nanometers across plays a dominant role in many natural and technological processes ranging from clay swelling, frost heave, and catalysis via colloidal stability and protein folding to transport across artificial nanostructures and bio-membranes. In nanoporous media the geometrical confinement and pore wall-fluid interactions as well as complex pore morphologies may significantly alter water's physico-chemical equilibrium and non-equilibrium properties, causing, for example, the molecular structuring of the fluid, huge negative Laplace pressures in the liquid and changed shear viscosities.



Laser-ultrasound experiment on water-infiltrated nanoporous silicon. (TUHH/DESY/Künsting)

In the first part of my talk I will present opto-fluidic, X-ray and neutron scattering experiments on capillarity-driven transport, self-diffusion dynamics of water and aqueous electrolytes in nanoporous solids [1, 2] as well on the interplay of water's capillarity with the confining solids' elasticity [3, 4]. The observations on the effective, porous-medium scale will be related to the single-nanopore fluid properties [2], also by resorting to computer simulations. In the second part of my talk I will exemplify that exploiting water's peculiar nanofluidics in com-bination with self-organized porosity in solids offers an entirely novel design space for sustainable, active integrated materials with functional diversity. In particular, I will present porous materials with electrically switchable wettability and hydraulic permeability [5] as well as large electrochemo-mechanical actuation for potential applications in Lab-on-a-Chip fluidics, sensorics, water filtration and energy conversion [5,6].

References:

[1] Capillary rise of water in hydrophilic nanopores. S. Gruener and T. Hofmann and D. Wallacher and A.V. Kityk, P. Huber, Phys. Rev. E 79, 067301(2009).
[2] Dynamics of water confined in mesopores with variable surface interaction. A. Jani, M. Busch, J.B. Mietner, J.Ollivier, M.Appel, B. Frick, J.M. Zanotti, P. Huber, M. Fröba, D. Morineau. J. Chem.Phys.154, 094505 (2021).
[3] Elastic response of mesoporous silicon to capillary pressures in the pores. G.Y. Gor, L Bertinetti, N. Bernstein, T Hofmann, P. Fratzl, P. Huber, Appl. Phys. Lett. 106, 261901 (2015).
[4] Laser-excited elastic guided waves reveal the complex mechanics of nanoporous silicon.M. Thelen, N. Bochud, M. Brinker, C. Prada, P. Huber, Nat. Comm. (2021, in press).
[5] Switchable imbibition in nanoporous gold, Y. Xue, J. Markmann, H. Duan, J. Weissmüller, P. Huber, Nat. Comm.5, 4237 (2014).
[6] Giant electrochemical actuation in a nanoporous silicon-polypyrrole hybrid material. M. Brinker, G. Dittrich, C. Richert, P. Lakner,

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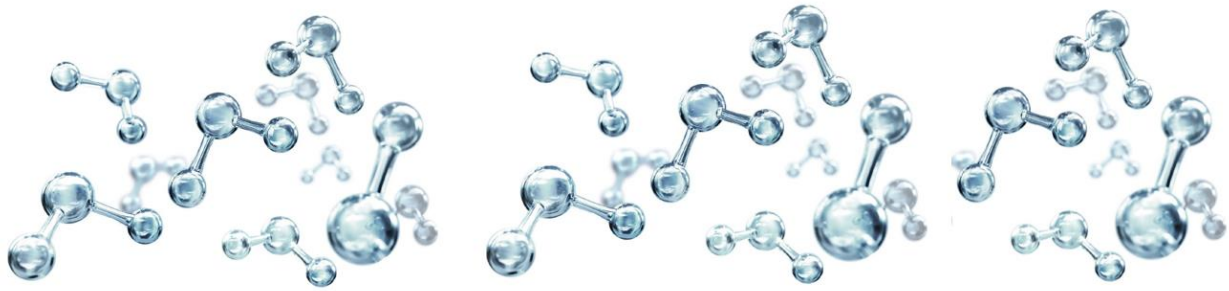


T. Krekeler, T.F. Keller, N. Huber, P. Huber. Sci. Adv. 6 eaba1483 (2020).

27th of May 2021
12:00 h

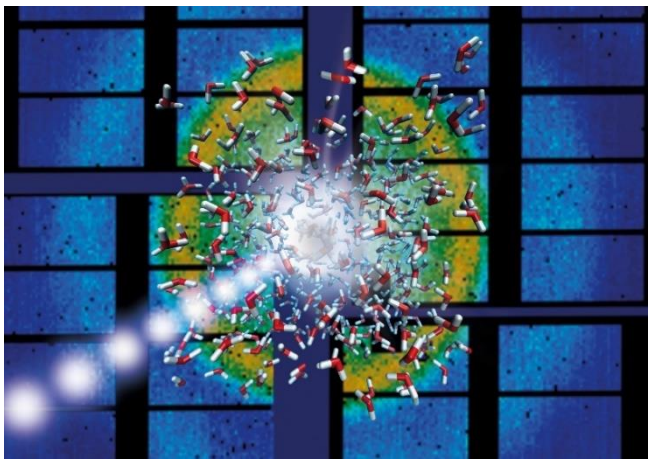
Felix Lehmkühler

Deutsches Elektronen-Synchrotron (DESY)

Probing nanoscale dynamics with MHz repetition rates – superheating water above 170 °C

Dynamics and kinetics in soft-matter physics, biology, and nanoscience frequently occur on (sub-) microsecond time scales, which are difficult to probe experimentally. One way to access dynamics over multiple length scales is X-ray photon correlation spectroscopy (XPCS) using coherent X-rays. In particular, the European XFEL enables XPCS experiments down to atomic length scales for the first time thanks to its MHz repetition rate.

In this talk I will first introduce the concept of XPCS. Afterwards I will present the results of microsecond XPCS at the SPB/SFX instrument of European XFEL on the dynamics of nanoparticles dispersed in water [1]. We found an exceptional beam stability over the pulse train, suggesting very weak—if any—shot-to-shot fluctuations of beam size, pointing, and coherence. By fine-tuning the fluence of the European XFEL pulses, we were able to observe different degrees of beam-induced heating of both the nanoparticles and the surrounding water. At fluences above 50 µJ/mm2, superheated-water states above 170°C were reached, which persisted at least for 100 µs. At the end of the talk I will give a short outlook on the possibilities of XPCS experiments at the next-generation X-ray light sources.



[1] F. Lehmkühler et al. PNAS 117, 24110 (2020).