CPP 19: Focus Session: Water – from Atmosphere to Space I (joint session CPP/DY)

Water plays a vital role in diverse Earth processes across multiple scales, from atmospheric cycles and aerosol chemistry to geological porous media and nanoscale biological functions of hydrated proteins. Despite its fundamental importance and numerous anomalous properties, such as the diverging heat capacity of supercooled water, pure bulk water remains poorly understood. Key phenomena like evaporation and crystallization are relevant not only on Earth but also in extraterrestrial environments. In Germany, molecular water research is flourishing across prestigious centers, exemplified by the new BlueMat cluster at Hamburg University of Technology, the renewed RESOLV cluster at Ruhr-University Bochum, and the Max Planck Society's expanding Liquid Initiative in Mainz. The 2025 inauguration of the Centre for Molecular Water Science (CMWS) at Hamburg's DESY campus further strengthens a Europe-wide interdisciplinary network, uniting 47 founding members from 12 countries to advance water science across disciplines and methods. Within this focus session the state of molecular water research shall be discussed and interactions between the physical sub-fields shall be fostered.

Organized by Alexander Schlaich, Katrin Amann-Winkel, Mischa Bonn.

Time: Tuesday 9:30–11:00 Location: ZEU/LICH

Topical Talk CPP 19.1 Tue 9:30 ZEU/LICH

Surface adsorption and protonation equilibrium of atmospheric organics at the aqueous surface — •Nønne Prisle — Center for Molecular Water Science, Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, D-22607 Hamburg, Germany — Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany — Center for Atmospheric Research, University of Oulu, P.O. Box 4500, FI-90014, Oulu, Finland

Atmospheric aerosols comprise a significant fraction of organic species which frequently exhibit both surface activity and Brönsted acidity or basicity in aqueous solutions. The high surface area to bulk volume ratios of nano- and microscopic aerosols and droplets further favor surface-specific states, affecting both bulk-phase and heterogeneous chemistry.

We used X-ray Photoelectron Spectroscopy (XPS) in combination with high-brilliance synchrotron radiation to directly observe the protonation state of atmospheric acids and bases at the surfaces of aqueous aerosol and droplet models. We found that for each acid-base pair, the neutral species is enhanced in the surface, consistent with its higher surface activity, compared to the charged conjugate. This introduces a shift in the protonation equilibrium at the aqueous surface corresponding to an apparent change in pKa of 1-2 pH units, depending on the concentration, acidity, and surface activity of the conjugate acidic and basic species.

CPP 19.2 Tue 10:00 ZEU/LICH

The Effect of pH on the Structure of Model Sea Spray Aerosol Surfaces — •Clara M. Saak, Lars Höhner, and Ellen H.G. Backus — Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Währinger Straße 42, 1090 Vienna, Austria

Aerosols play a key role in the global climate due to their ability to scatter and reflect solar radiation and to act as cloud condensation nuclei (CCN), exerting a pronounced cooling influence on the global climate. In particular, the surface availability of ions and organic compounds is known to affect the hygroscopicity of the particle and thereby its ability to act as a CCN [1]. While the surface propensity of individual compounds has been studied widely, much less is known about more complex systems. Here we focus on the impact of bulk pH on the architecture of mixed aqueous interfaces. In atmospheric systems the pH has been shown to range from roughly pH 8 to 2 [2]. Using sum-frequency-generation (SFG) spectroscopy in conjunction with surface tension data we study the surface composition and structure of short and long chain organic acids at different protonation stages, obtained by varying the pH. Using this approach, we find pronounced changes in the structuring of the aqueous sub-surface layers depending on the specific composition and pH, and in the Gibbs free energy of adsorption of the studied organics. Our results show that it is feasible for subtle environmental changes to considerably affect structure and composition of the aqueous interface, which is known to play a key role in aerosol hygroscopicity. [1] Zieger, Nat. Commun. 2017, 8, 15883. [2] Angle, PNAS, 2021, 118, 2, e2018397118

CPP 19.3 Tue 10:15 ZEU/LICH

Crystallization behaviour of nanoparticle suspensions — •Isabell Zick[1,2], Eduard Edel[2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, 55128 Mainz, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Water is one of the most abundant substances in the world and due to this in close contact with many materials including micro- and nanoplastic particles. Those have been detected not only in sea but also in the atmosphere, where the particles can interact with water and act as cloud condensation nuclei or ice-nucleating particles. Emerging evidence suggests that nanoparticles with increased surface roughness or chemical functionalities may promote heterogeneous ice nucleation through different processes like, e.g., contact- and immersion-freezing. Such a behaviour affects cloud properties with significant implications for Earth*s radiative balance and the hydrological cycle.

We investigate atmospherically relevant nanoparticles dispersed in water to investigate their influence on the ice crystallization. Our experiments include calorimetry (DSC) as well as X-ray diffraction measurements (XRD). Our measurements show that the crystallization temperature depends on the particle size, concentration, and the chemical surface of the particles. Using XRD, we investigate the restructuring of the water molecules during supercooling, observed by a shift in the characteristic main diffraction peak of water and the subsequent crystallization process.

CPP 19.4 Tue 10:30 ZEU/LICH

Laser-Excited X-ray Reflectivity of Aqueous SrCl2 at the Air-Water Interface — •Ali Ashtiani Abdi[1,2], Julia Kobus[1,2], Svenja C. Hövelmann[1,2], Philipp Jordt[1,2], Nicolas Hayen[1,2], Prashant Hitaishi[1,2], Ajay Ajay[1,2], Rabia Qamar[1,2], Otto Lippmann[1,2], Chen Shen[3], Florian Bertram[3], and Bridget M. Murphy[1,2] — [1]IEAP, CAU Kiel University, Kiel, Germany — [2]Ruprecht Haensel Laboratory, DESY, Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Understanding aqueous interfaces is essential for describing chemical processes in atmospheric, marine, and geochemical environments. While monovalent salts have been widely studied, the interfacial behavior of divalent ions is less understood, despite their relevance in seawater aerosols and reactive brines. SrCl2 is a representative divalent electrolyte whose interfacial structure may show alteration by laser illumination.

We investigate aqueous SrCl2 solutions at different concentrations using X-ray reflectivity (XRR) at the liquid-air interface. Measurements were performed at the LISA setup at beamline P08, PETRA III (DESY), where controlled laser illumination can be applied directly to the X-ray footprint, following the instrumentation concept of Warias and Hovelmann et al. (J. Synchrotron Rad. 2024). Reflectivity curves were recorded with and without laser exposure. The data demonstrate the suitability of SrCl2 surfaces for laser-assisted XRR and the sensitivity of the method to potential changes in interfacial structure, including indications of near-surface layering.

CPP 19.5 Tue 10:45 ZEU/LICH

Monitoring Uptake, Release and Reaction of Gases at the Liquid-Vapor Interface — •Tillmann Buttersack[1], Shirin Gholami[1], Clemens Richter[1], Daniela Torres-Diaz[1], Bernd

Winter[1], Pavel Jungwirth[2], Stephen Bradforth[3], Markus Ammann[4], Ruth Signorell[5], Ivan Gladich[6], Remi Dupuy[7], Philip Mason[2], and Hendrik Bluhm[1] — [1]Fritz Haber Institute, Max Planck Society, Berlin, GER — [2]IOCB, Czech Academy of Sciences, Prague, CZ — [3]University of Southern California, Los Angeles, USA — [4]Paul Scherrer Institut, Villigen, CH — [5]EZH Zürich, CH — [6]University of Urbino, Urbino, I — [7]Sorbonne Université, Paris, F

Multiphase reactions are omnipresent in nature, industrial applications. The direct observation of reactions at the liquid-vapor interface requires spectroscopic techniques that are surface specific and chemically sensitive to detect low concentrations, e.g., photoelectron spectroscopy (XPS). Furthermore, the sample delivery method must allow sufficient time for an interface reaction to proceed. These complex challenges require individual approaches for each system of interest. One example for a multiphase process is the reaction between liquid alkali metal and water vapor, which is extremely fast. We used a slow droplet train of NaK in a wet atmosphere and observed the formation of golden aqueous solutions with metallic properties with XPS. An example with relevance for atmospheric chemistry is the formation and the release of sulfur dioxide (SO2) from aqueous sulfite solutions due to acidification. We demonstrated that dissolved gases can be detected with XPS even though their concentration is only about 1 mM.