CPP 32: Focus Session: Water – from Atmosphere to Space IV (joint session CPP/DY)

Time: Wednesday 9:30–10:45 Location: ZEU/0260

Topical Talk CPP 32.1 Wed 9:30 ZEU/0260

Synchrotron X-Ray Studies on Structural Transitions in Water and Alcohol containing Ice Analogues — •Christina M. Tonauer — Institute of Physical Chemistry, University of Innsbruck, Austria — Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

To this date, 21 different crystalline and at least 3 distinct amorphous forms of water ice have been discovered. In addition to the structural versatility of pure water ice phases, water forms solid guest-host systems, so-called 'clathrate hydrates' where water builds cage-like structures around guest molecules of various sizes (e.g., Ar, CO2, methane, ethanol).

Ices in space are exposed to various forms of (external) stress, e.g., impacts, cosmic rays, UV/Vis radiation as well as endogenous thermal fluctuations, thereby undergoing structural changes. By studying such structural transitions in ice analogues upon heating (and/or radiation), conclusions can be drawn about the conditions at various extraterrestrial environments.

Therefore, we here present temperature-resolved wide- and small-angle synchrotron X-ray scattering data of vapor-deposited water-ethanol mixtures of various concentrations, collected at PETRA 3/DESY. While the SAXS data allows for monitoring of changes of the morphology of the microporous sample, the WAXS data reveals the formation sequence of two different hydrates, offering new insights into the crystallisation of astrophysical ices.

CPP 32.2 Wed 10:00 ZEU/0260

Water in exoplanetary atmospheres: from molecular spectra to Water Worlds — •Sergey Yurchenko — Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT London, United Kingdom

Water vapour is one of the key tracers of atmospheric physics and chemistry on exoplanets, from hot Jupiters to temperate sub-Neptunes and so-called Water Worlds. In this contribution I will give an overview of the role of H_2O across this diversity of atmospheres, focusing on how we infer its presence from transmission and emission spectra. I will review both low-resolution transit spectroscopy and high-resolution cross-correlation techniques, and show how they are applied to data from space- and ground-based facilities, including JWST, Hubble and VLT, as well as future observations with the ELT and ESA's Ariel mission. Special emphasis will be placed on the way clouds and hazes imprint themselves on the observed spectra.

I will summarise the current observational status of water detections and non-detections – including recent and sometimes controversial claims for habitable-zone planets. A central theme of the talk will be the importance of accurate laboratory and theoretical data for water and related species. I will highlight how comprehensive molecular line lists and cross sections from the ExoMol and HITRAN databases, together with other laboratory measurements, underpin the modelling and retrieval of exoplanet spectra over a wide range of temperatures, pressures and compositions, thereby linking detailed molecular physics to the emerging picture of water in exoplanetary atmospheres.

CPP 32.3 Wed 10:15 ZEU/0260

Structures of Ices by Quantum Crystallography and PDF — Krzysztof Wozniak[1], •W. Sławiński[1], G. Łach[2], R. Gajda[1], M. Chodkiewicz[1], P. Rejnhardt[1], M. Arhangelskis[1], Ch. Ridley[3,4], and C. L. Bull[3,5] — [1]Deptm. of Chem., Univ. of Warsaw,Poland — [2]Deptm. of Phys., Univ. of Warsaw, Poland — [3]ISIS Neutron and Muon Source, STFC, RAL, Harwell Campus, UK. — [4]Spallation Neutron Source, Oak Ridge Nat. Lab., Oak Ridge, Tennessee 37830, USA — [5]Univ. of Edinburgh, UK.

Ice is the solid form of water (H*O). The most familiar form of ice is the hexagonally structured ice Ih. However, water can crystallize into at least 21 distinct phases, unique in structure, depending on T and P and route of formation. In this contribution, will present details of structures of ices (VI[3], VII[1,2], Ih [4]) obtained with quantum-crystallographic Hirshfeld Atom Refinement against single crystal X-ray and electron diffraction data. We will also present the first quantitative characterisation of disorder in D2O ice VII and VI obtained through a combination of Pair Distribution Function (PDF) analysis, Reverse Monte Carlo (RMC) modelling, and high-pressure neutron scattering. Our results provide a detailed decomposition of both the average and local atomic structures of Ice VII, revealing a previously unquantified level of structural disorder. References [1] R. Gajda et al., IUCRJ, 12(3) (2025) 288-294; [2] W. A. Sławiński et al., Hidden complexity in D2O Ice VII, Acta Mat., (2025) submitted; [3] M. L. Chodkiewicz et al., IUCRJ, 9 (2022) 573-579; [4] M. L. Chodkiewicz et al., IUCRJ, 11(5) (2024) 730-736.

CPP 32.4 Wed 10:30 ZEU/0260

Water dynamics in conductive PEDOT:PSS/cellulose nanocomposite films in dependence of relative humidity and temperature — •Lucas Kreuzer[1], Marie Betker[2], Marcell Wolf[1], Jacques Ollivier[3], Daniel Söderberg[4], and Stephan V. Roth[2,4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [2]Deutsches Elektronen Synchrotron, Hamburg, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Engineering Mechanics, Royal Institute of Technology KTH, Stockholm, Sweden

PEDOT:PSS is a conductive and water-soluble polymer blend widely used in organic electronics. However, pure PEDOT:PSS films absorb significant amounts of water, causing swelling, degradation, and eventually a decrease in conductivity. Integrating PEDOT:PSS with cellulose nanofibrils (CNFs) overcomes these issues by limiting water absorption and enhancing mechanical stability. However, a minor amount of water is still absorbed, leading to a change in film morphology: high humidity induces de-wetting of PEDOT:PSS from the CNFs, reducing conductivity, whereas drying generally leads to a re-wetting of PEDOT:PSS, thereby restoring conductivity. To investigate further the role of water, quasi-elastic neutron scattering is applied, which reveals two water species in the films: mobile bulk water and slower hydration water. Upon drying, bulk water is released completely, while hydration water remains in the films, supporting the re-wetting of PEDOT:PSS. Moreover, at higher temperatures, different diffusive behavior was found for bulk and hydration water.