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► **To cite this version:**

Mihail Barboiu, Barbara Kirchner, Eva Perlt, Alessandro Scarso. H 2 Open – Guest Editorial. ChemistryOpen, 2023, 10.1002/open.202300072 . hal-04257813

**HAL Id: hal-04257813**

**<https://hal.science/hal-04257813>**

Submitted on 25 Oct 2023

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## H<sub>2</sub>Open – Guest Editorial

Mihail Barboiu,<sup>\*,[a]</sup> Barbara Kirchner,<sup>\*,[b]</sup> Eva Perlt,<sup>\*,[c]</sup> and Alessandro Scarso<sup>\*,[d]</sup>

This special collection presents original research articles and reviews that are connected to the multifaceted and rich chemistry of water. These works serve as an illustration of how, despite its apparent simplicity and ubiquity, water continues to

be at the center of scientific exploration from a wide range of perspectives and employing the toolbox of modern-day chemistry.

Solvent, reagent, catalyst, impurity, electrolyte, drink, ligand, and much more – water can be anything but ordinary. It is therefore not surprising that this substance continues to be the matter of active high-quality research. Its outstanding role amongst other solvents is due to certain unusual properties such as its self-dissociation, which gives rise to the whole field of acid-base chemistry and the concept of pH, the proton transfer mechanism through Grotthuss diffusion, its irregular phase diagram featuring a density maximum and a large number of solid phases, or its exceptionally high heat capacity, to name only few. The list gets even longer if other factors are taken into account such as the classical and non-classical hydrophobic effect giving rise to confinement effects or interface phenomena, solvated ions or molecules, or excitation by electromagnetic fields in spectroscopy. The fact that water stands out in so many ways makes it at the same time a very popular field of research and an extremely challenging one.

In this collection, we have assembled review and research articles that shed light on water from different viewpoints covering thermal response properties, catalysis, nanoparticles, global polarity, dynamics, supramolecular chemistry, and cav-

itands in water. The broad field of applied methods ranging from thermal measurements via synthesis to NMR spectroscopy and computer simulations—the latter one ranging from path-integral simulations to coarse-grained models—demonstrates how versatile this inconspicuous three-atomic molecule and its properties are.

In their research article, Shengjun Du and co-workers study the adsorption kinetics of water in microporous C<sub>2</sub>N-type carbon materials with potential applications for water storage and thus, providing potable water in arid regions. Using thermal response measurements, the authors demonstrate how the water adsorption dynamics can be enhanced by decreased particle size, which in turn can be achieved by ball milling.

Ana Paula Nazar de Souza and colleagues present how water can act as a solvent in organic synthesis at mild conditions paving the way to more sustainable, less toxic, and hence, environmentally friendly synthetic routes. The authors demonstrate how light activation and a bimetallic catalyst can result in excellent yields using water as a solvent at ambient temperature for Suzuki–Miyaura reactions.

Another step towards sustainable synthetic chemistry is taken by Luciana Cicco et al., who present the selective oxidation of alcohols in water and low melting mixtures. The copper/TEMPO catalyzed reaction protocol provides another example for a more sustainable synthesis using water or a biodegradable low melting mixture and operating at ambient temperatures.

A more mechanistic research article is provided by Stefan Spange and co-workers, who investigate the global polarity of water and alcohols as hydrogen bond donating solvents. Three different effects are considered to investigate this property and implications for the characterization of the hydrogen bond donating character of these solvents are given.

The effect of polarity on the molecular conformation of a solute molecule is studied by Anjali Gaur and Sundaram Balasubramanian. Through atomistic molecular dynamics simulations using an accurate force field for ethylene glycol/water mixtures at various mole fractions they unraveled this interaction between solvent polarity and solute conformation and the influence on various properties.


Nazrollah Rezai-Ghaleh presents water dynamics from another perspective using multi-nuclear NMR spectroscopy to


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 This publication is part of a Special Collection of ChemistryOpen including invited contributions focusing on the multifaceted chemistry of water - H<sub>2</sub>Open.

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investigate the dynamics of water in highly concentrated (saturated) salt solutions. It is observed that water molecules maintain a high mobility in saturated salt solutions, in particular potassium chloride, which is relevant for example in compartments of high ion concentration in living cells.

A theoretical study on non-linear optical processes at the vacuum-water interface is provided by Tárcius N. Ramos and Dr. Benoît Champagne. They apply elaborate multi-scale modeling to study the second harmonic generation at and near the

interface, which is relevant in atmospheric, biological, and organic chemistry, amongst others.

The special role of light hydrogen atoms in the hydrogen bond network, which involves a significant amount of nuclear quantum effects, is accounted for by a novel variant path integral molecular dynamics simulations in a reservoir contributed by Antonios Evangelakis et al. This method allows such accurate simulations on a scale that has been infeasible before



Mihail Barboiu graduated from University Politehnica of Bucharest and received his PhD in 1998 from the University of Montpellier. He is CNRS Research Director at the Institut Europeen des Membranes in Montpellier and Fellow of Royal Society of Chemistry. A major focus of his research is Dynamic Constitutional Chemistry toward Dynamic Interactive Systems: adaptive biomimetic membranes, delivery devices etc. Author of more than 340 scientific publications and 450 conferences and lectures, Dr Barboiu has received the EURYL Award in Chemistry in 2004 and the RSC Surfaces and Interfaces Award in 2015 for the development of Artificial Water Channels.



Barbara Kirchner holds a chair for theoretical chemistry at the Mulliken center for Theoretical Chemistry in Bonn. She is a member of the trans-disciplinary research areas "Building Blocks of Matter and Fundamental Interactions" and "Innovation and Technology for Sustainable Futures" at the University of Bonn. Furthermore, she serves as Editor of Topics in Current Chemistry and as a senior editor for the ACS Journal of Physical Chemistry after serving for Chemical Physics as editor. She is specialized in theoretical methods for liquids, for example ionic liquids and deep eutectic solvents. However, her research interests and impact reach far beyond the topic of ionic liquids, they cover a wide range of fields in theoretical, physical, (bio)organic, inorganic and sustainable chemistry. She investigates functional materials such as chemically active domains in liquids, bulk and interfacial liquid-liquid systems for extraction, and energy devices. Her research involves two larger software projects: Peacemaker and Travis. While the former program is gradually gaining more and more attention for predicting physical and chemical properties of liquids based on high level quantum chemical calculations, the latter allows a systematic characterization of molecular simulation trajectories, and is used broadly in the international scientific community. In 2017 she held the Inman Lecture of the Molten Salts and Ionic Liquids Discussion Group of Royal Society of Chemistry (UK). In 2019 she was awarded the Ruth Lynden-Bell Award at the ILMAT V in Paris (France) and in the same year she was an Invited Professor of the University of Strasbourg (France).



Eva Perlt graduated from the University of Leipzig where she also completed her PhD in 2014. After research stays at the University of Bonn, the University of California, Irvine, and the Free University Berlin, she is currently a Junior Research Group Leader at the Otto Schott Institute for Materials Research at the Friedrich Schiller University Jena (since 2021). Her research is focused on the role of nuclei in electronic structure calculations. In that context, she studies nuclear quantum effects as well as vibrational data beyond the harmonic approximation.



Alessandro Scarso is professor of Organic Chemistry at Università Ca' Foscari Venezia. He holds a PhD in Chemical Sciences and Laurea Degree cum Laude from Università di Padova. He spent a two year post-doc in the group of prof. Rebek at Scripps Research Institute (La Jolla, CA) working on organic self-assembled capsules for selective recognition and catalysis. He is co-author of more than 90 articles and reviews in international peer-reviewed journal and 20 book chapters. He received awards for studies in catalysis (2015, Gian Paolo Chiusoli Medal, Industrial division, Società Chimica Italiana), (2012, Istituto Italiano Scienze e Lettere), (Young Scientist, Università Ca' Foscari, 2010). He is member of the editorial board of *Organics* and *Frontiers in Chemistry* (section supramolecular chemistry). His interest spans from the development of new scaffolds for supramolecular self-assembly of nanocontainers, to supramolecular catalysis in water and organic media, synthesis of bioactive compounds and sustainable synthesis of drugs in collaboration with pharma companies.

and will result in new insights into the structure and dynamics of water's liquid phase.

In a comprehensive review article, Stefan Kubik discusses the solvent effect of water with regard to molecular recognition. Due to the complexity of the interactions in water, a fundamental understanding of its role in molecular recognition is still lacking. In this review, different types of interactions between substrate and receptor are introduced and an overview about the respective receptors is given, thereby shedding light on this complex matter.

Such molecular recognition processes can be used to bind pollutants in water. In the review article by Yu Jie Zhu, water-soluble cavitands are introduced which can be applied not only for the removal of organic pollutants, but also for guest separations or as reaction vessels.

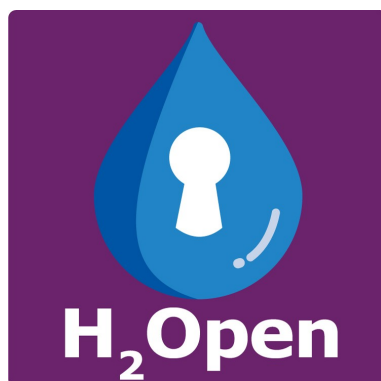
We are delighted by the broad range of research areas, from which articles have been contributed, ranging from fundamental method development in the field of simulations to synthesis and macro-molecular chemistry, which once more emphasizes the versatility and the numerous challenges for experiment and theory of this extraordinary substance. We hope you enjoy the read.

### ***Conflict of Interest***

The authors declare no conflict of interest.

## EDITORIAL

**H<sub>2</sub>Open** is a special collection of research articles and reviews focused on the multifaceted chemistry of water from different scientific vantage points. Guest editors Mihail Barboiu, Barbara Kirchner, Eva Perlt and Alessandro Scarso give an overview of the collection.



*Prof. Dr. M. Barboiu\**, *Prof. Dr. B. Kirchner\**, *Dr. E. Perlt\**, *Prof. Dr. A. Scarso\**

1 – 4

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