CPP 34: Focus Session: Interactions Between Water and Cellulose I

Time: Thursday 15:00–16:00 Location: H34

Invited Talk CPP 34.1 Thu 15:00 H34

Understanding Nanocellulose-Water Interactions to Engineer Advanced Functional Materials — •Valentina Guccini — Uppsala University, Lägerhyddsvägen 1, Uppsala, Sweden

Water interactions are a central topic in the field of nanocellulose due to their pivotal role in nanocellulose's chemical reactivity, processability and physical properties. Yet, a key challenge that remains is bridging the fundamental understanding of nanocellulose-water interactions with the design and engineering of advanced functional materials. This presentation will address this challenge by summarizing the main characteristics of water-nanocellulose interactions and how these can be leveraged to engineer nanocellulose-based materials, in which water has both a structural and functional role. We will analyze the structure-property relationship in nanocellulose-based hydrogels, films and membranes for biotechnological and fossil-free energy applications (e.g. fuel cells and lithium-ion batteries). This presentation offers a new perspective on using nanocellulose-water interactions as a tool to enhance and tailor material performance and functionalities.

CPP 34.2 Thu 15:30 H34

Using Nanocellulose Hygroscopicity for Conductive 3D Paper Structures — •Marie Betker[1,2], Tim Erichlandwehr[3], Benedikt Sochor[1,4], Elisabeth Erbes[1,5], Yamit Alon[2], Alisher Kurmanbay[2], Yanan Li[6], Irene Fernandez-Cuesta[3], Peter Müller-Buschbaum[6], Simone Techert[1,5], Daniel Söderberg[2,7], and Stephan Roth[1,2,7] — [1]Deutsches Elektronen Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, Teknikringen 56, 10044 Stockholm, Sweden — [3]Hamburg Advanced Research Centre for Bioorganic Chemistry, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [4]Lawrence Berkeley National Laboratory, 6 Cyclotron Rd, Berkeley, CA 94720, USA — [5]Institute for X-ray Physics, Goettingen University, Friedrich Hund Platz 1, 37077 Göttingen, Germany — [6]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [7]Wallenberg Wood Science Center, Teknikringen 52, 10044 Stockholm, Sweden

We report the fabrication of the, to this date, thinnest sprayed nanopaper foils. For that, we spray aqueous nanocellulose dispersions layer-by-layer on a hot substrate. The foils are only 2 um thin with an average basic weight of 1.9 g/square metre. We specifically exploit the hygroscopicity of paper-based materials to rearrange our water-soaked foils into three-dimensional, free-standing shapes. We further demonstrate the applicability of our foils by making them conductive via integration of silver nanowires. This approach is a step towards more sustainable, 3D organic electronics.

CPP 34.3 Thu 15:45 H34

A simulation study of the structure and mechanical properties of cellulose and callose hydrogels — •Robinson Cortes-Huerto[1], Nancy C. Forero-Martinez[2], and Pietro Ballone[1] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, DE — [2]Institut für Physik, Johannes Gutenberg-Universität, Staudinger 9, 55128 Mainz, DE

The cell wall of plants is a complex, self-organized and continuously evolving structure playing important roles in the life cycle of individual cells and the plant as a whole. It consists primarily of cellulose, which is the main responsible for its mechanical properties. Under environmental stress, a crucial role is played by callose, a polysaccharide closely related to cellulose and a minority component of the cell wall. A recent study (*Plant Signal. Behav.* **2019**, *14*, e1548878) suggested that the enhancement of mechanical properties by callose is due to its ability to order neighbouring water molecules, giving origin to solid-like water-callose domains. This hypothesis is tested by atomistic MD simulations using models representing cellulose and callose hydrogels. The results highlight systematic differences in the coordination and H-bonding of callose and cellulose by water, reflected in different dynamical properties of water in callose or cellulose hydrogels, partly validating the hypothesis. However, mechanical properties, characterized by the Young's modulus of the polysaccharide / water gels, are the same in callose/ and cellulose/water samples, suggesting that callose's ability to link cellulose nanofibres into networks is the main responsible for the strengthening of the plant cell wall.