

# Capitalizing on Water Interactions

Tekla Tammelin

Industry meets FinnCERES

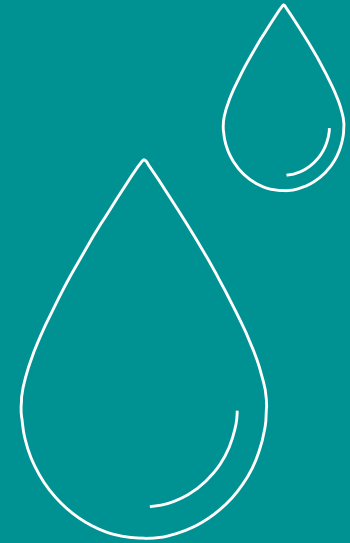
5<sup>th</sup> November, 2018



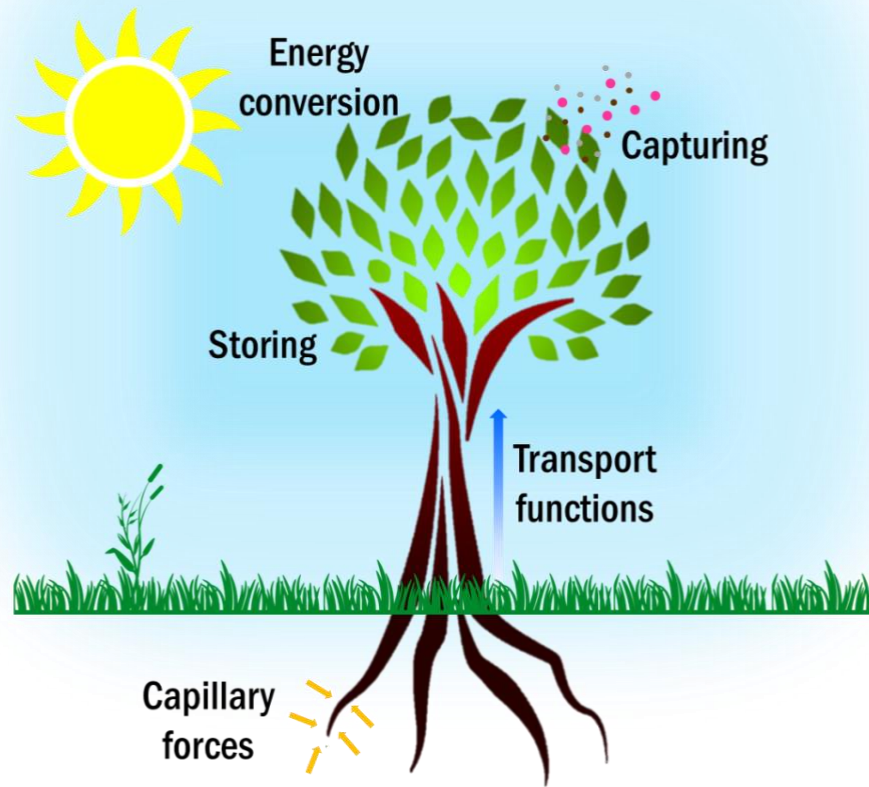
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**A!** Aalto University  
School of Chemical  
Engineering

**VTT**



# WATER INTERACTIONS ARE AT HEART OF BIOMATERIALS ENGINEERING



## *Plant cell wall functions based on water interactions*

- *Hygroscopic, hydrophilic, fiber swelling*
- *In applications water usually seen as a detrimental feature*

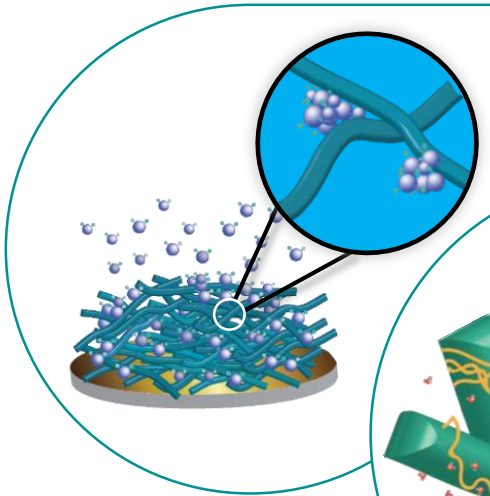
## *Water interactions define behaviour and mechanisms*

- *Biomass fractionation – isolation of the building blocks*
- *Reassembling structures – response to moisture and water*
- *Applications – draw inspiration from plant-based assemblies and functions*

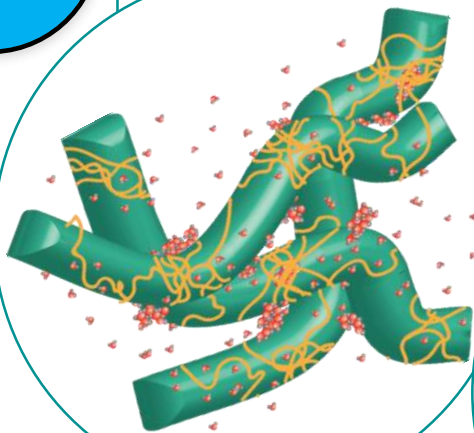
# APPLICATIONS – Turning challenge to **solution**

From basic discoveries towards applications

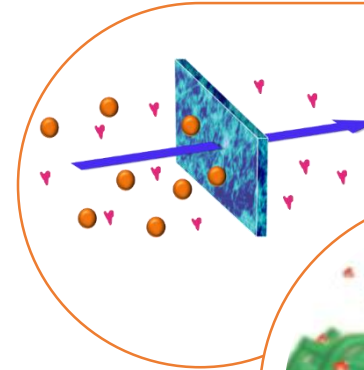
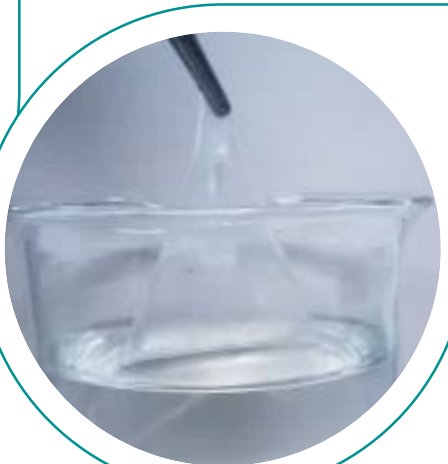
PRONOUNCED WATER UPTAKE ABILITY



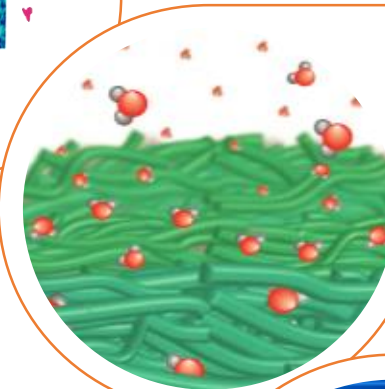
MOISTURE-RESPONSIVE STRUCTURES



ENHANCED WET STRENGTH

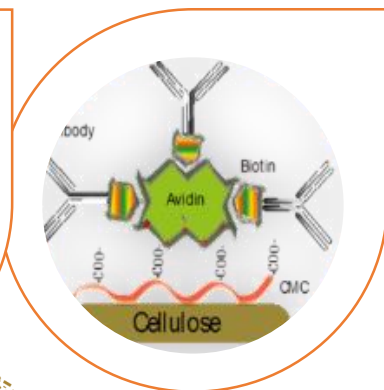


BIOINSPIRED CONCEPTS FOR WATER PURIFICATION  
– Capturing microplastics



GAS AND VAPOUR CAPTURING MATERIALS

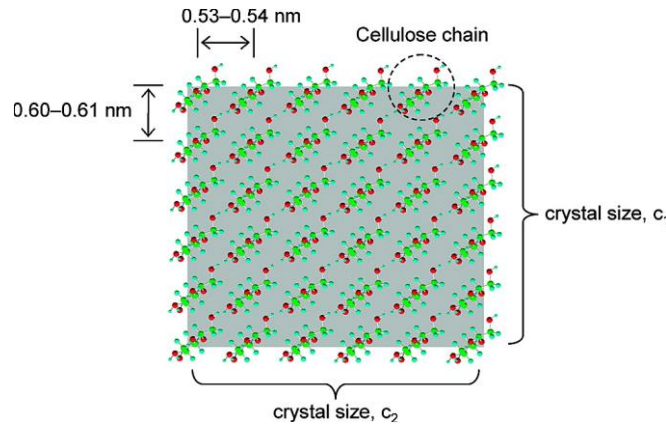
BIOBASED ELECTRONICS AND SENSOR ELEMENTS



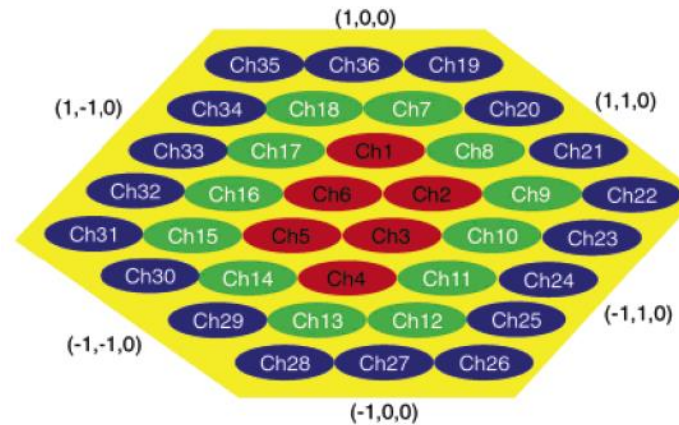
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# FUNDAMENTALS – Different models of cellulose microfibril structures under debate

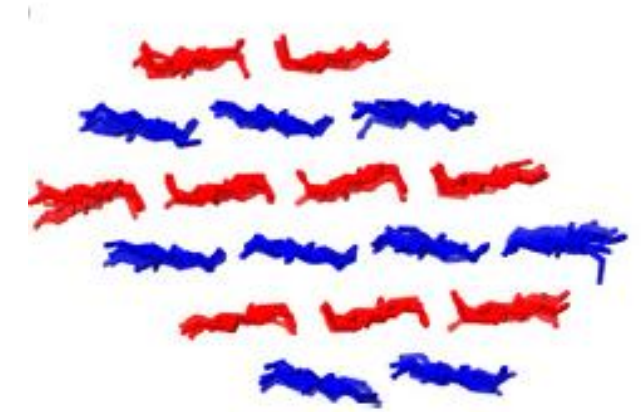
## CLASSIC 6×6 MODEL



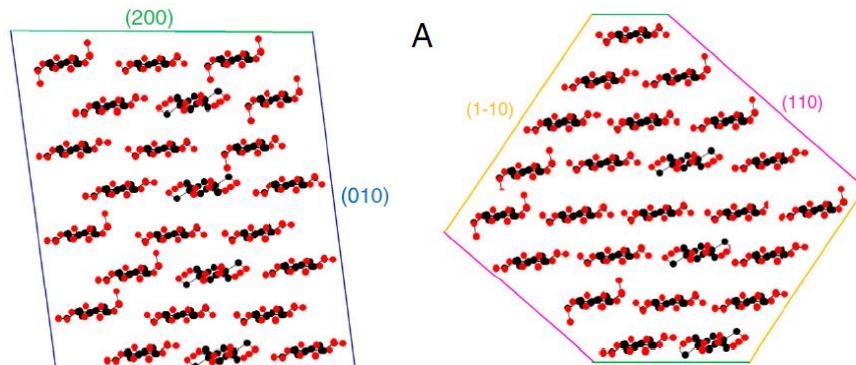
## ALTERNATIVE 6×6 MODEL



## 18 CHAIN MODEL



## 24 CHAIN MODELS



Ding and Himmel *J. Agric. Food Chem.* **2006**, 54, 597

Fernandes et al. *PNAS* **2011**, 108, E1195

Oehme et al. *Plant Physiol.* **2015**, 168, 3

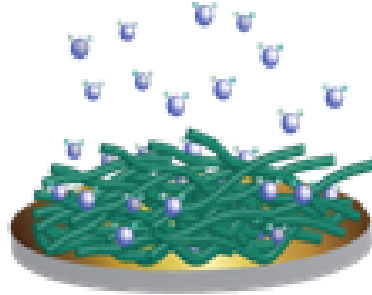
Endler and Persson *Mol. Plant.* **2011**, 4, 199

CONFIDENTIAL

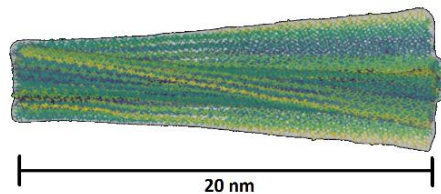


# OUR APPROACH: MAPPING THE DIMENSIONS VIA WATER SORPTION

- We can probe water interactions at interfaces with nanosensitivity and molecular level preciseness – *Surface sensitive methods*
- We can model the amount and location of water as well as structure of cellulose crystallites – *Molecular simulations*



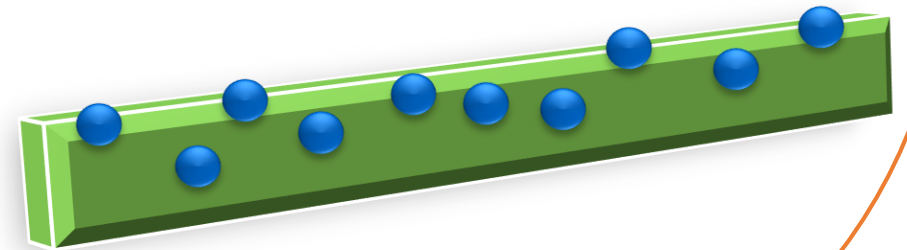
[Hakalahti et al.,  
Biomacromolecules (2017)]



[Ketoja et al., VTT-Aalto  
unpublished results (2018)]

**IDEA:** specific sites for water adsorption reveal details about the dimensions of cellulose crystal/microfibril

*Can we use water molecules to probe exact size and structure of the elementary microfibril?*



# THANK YOU!



**CERES**  
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**Eero Kontturi**  
Aalto University  
Professor

Internationally awarded expert in cellulose-based materials, particularly within the fundamental aspects of interfacial and surface-related phenomena.



**Tekla Tammelin**  
VTT  
Principal Scientist

Leading nanobiomaterial scientist with expertise in wide range of applications-related solutions rooted in science



**Zhuojun Meng**  
Joint post-doctoral  
researcher

Experienced scientist with strong background in biobased materials