From molecular structure to material properties: study of the chemical neighborhood of well-ordered and or chemical modified cellulose surfaces

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CNC with different sulphate content

MCC

Pulp

Side stream, hemicellulose extraktion

controlled acid hydrolysis

5x200 nm
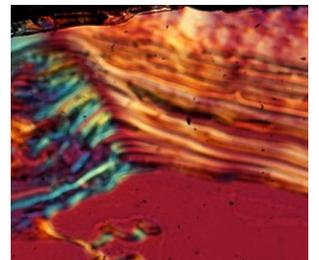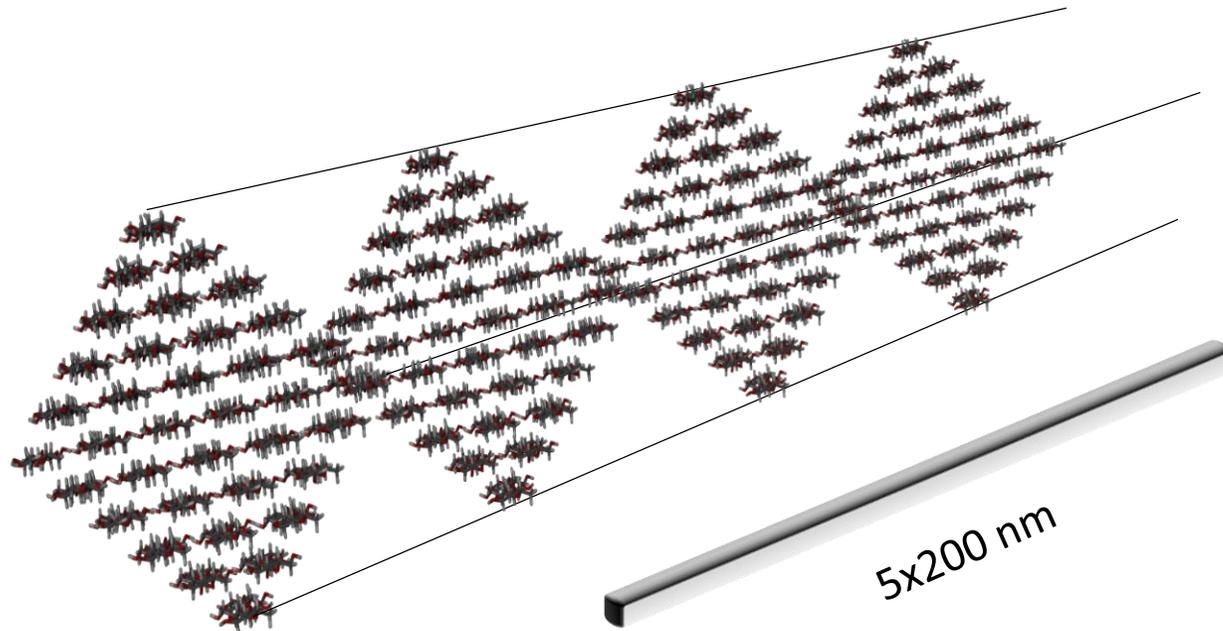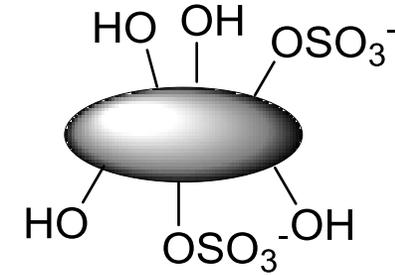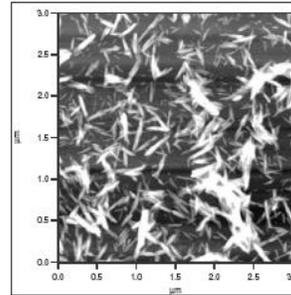
Chemical modification affect mesostructure
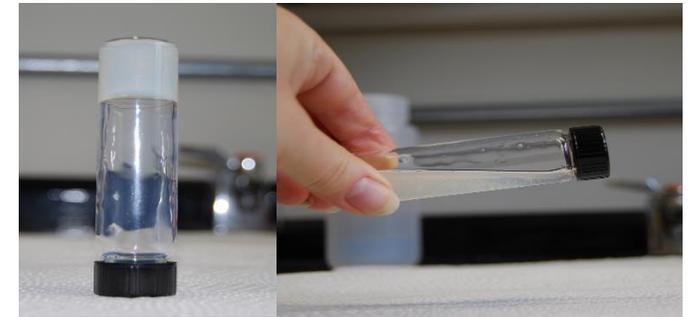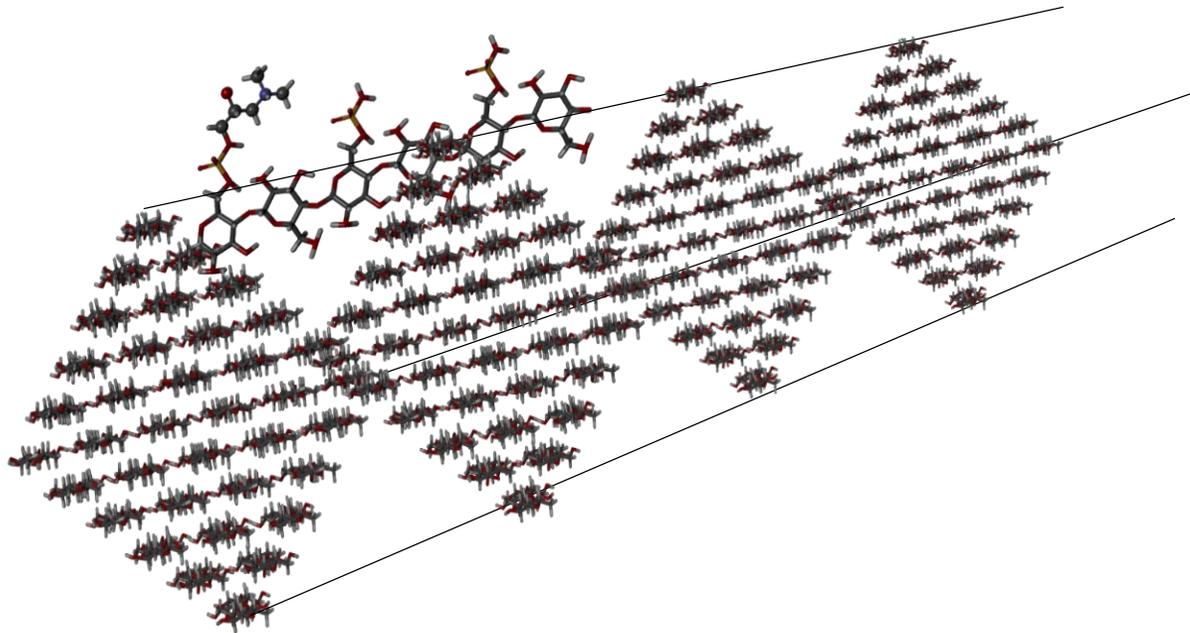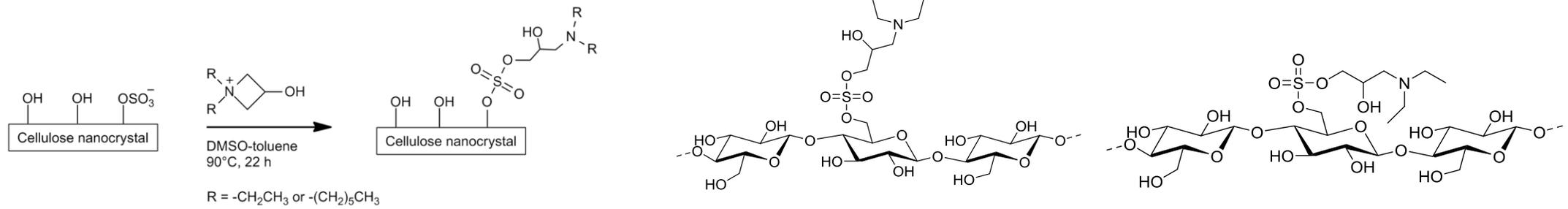
# Interface CNC particles and/or matrix

Shear thinning behaviour due to orientation of the CNCs.

The modified CNCs initially exhibit a gel-like behaviour.
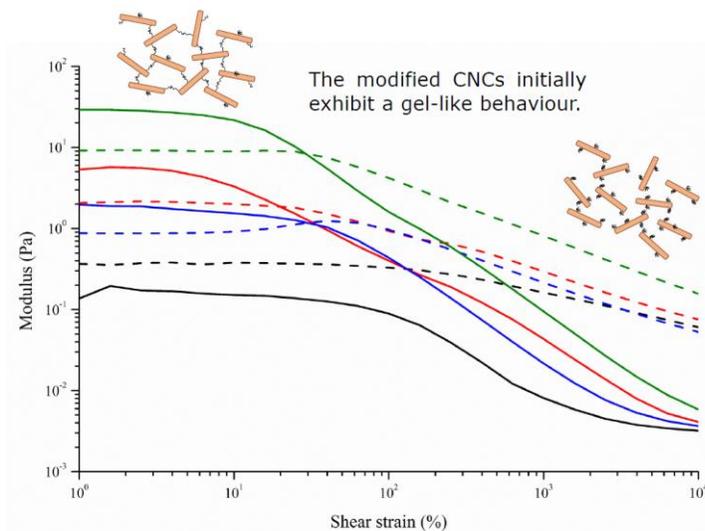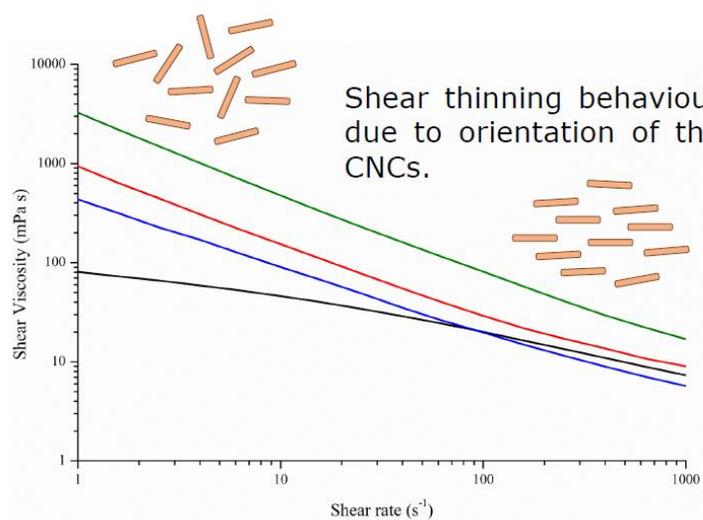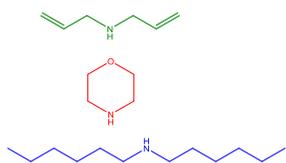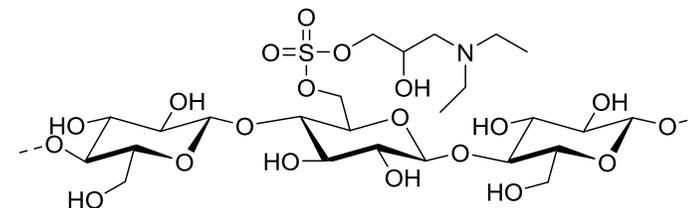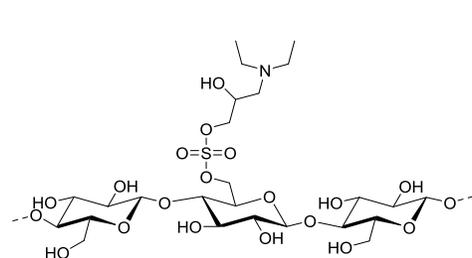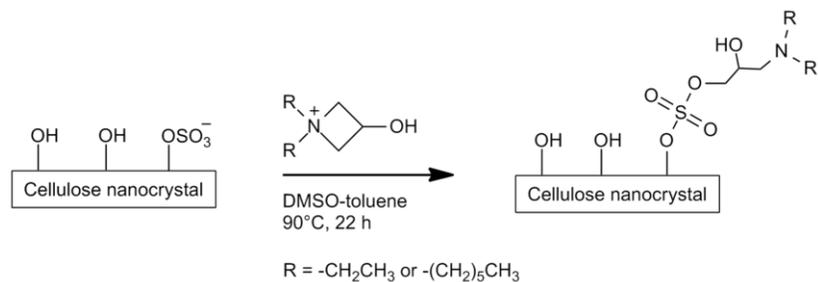
Flow curve for **unmodified CNC**, **CNC-Morph-Az**, **CNC-Dihex-Az** and **CNC-Diall-Az**.

Storage (——) and loss (— —) modulus for **unmodified CNC**, **CNC-Morph-Az**, **CNC-Dihex-Az** and **CNC-Diall-Az**.
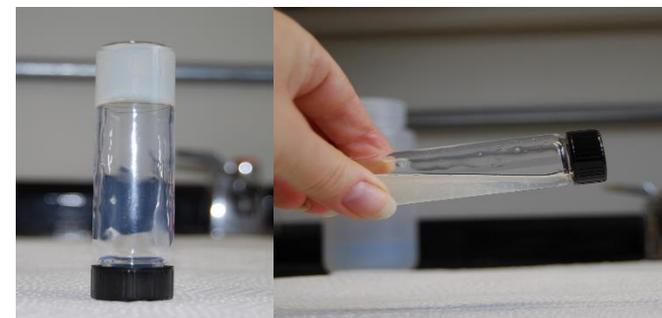
Hemicelluloses

L-arabino-4-O-methyl-D-Glucorono-D-Xylan

4-O-methyl-D-Glucorono-D-Xylan
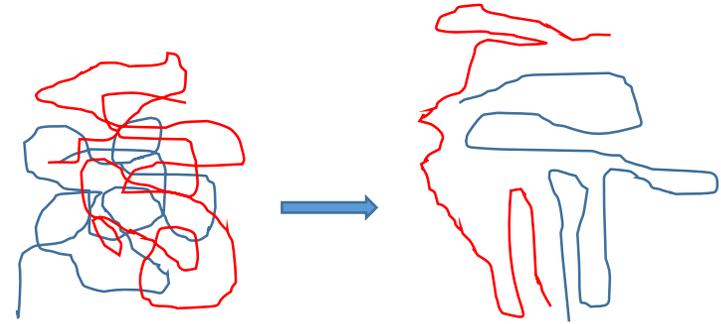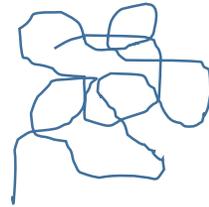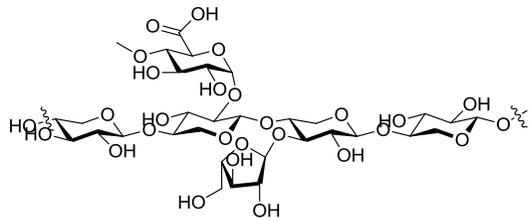
Galactoglucomannan
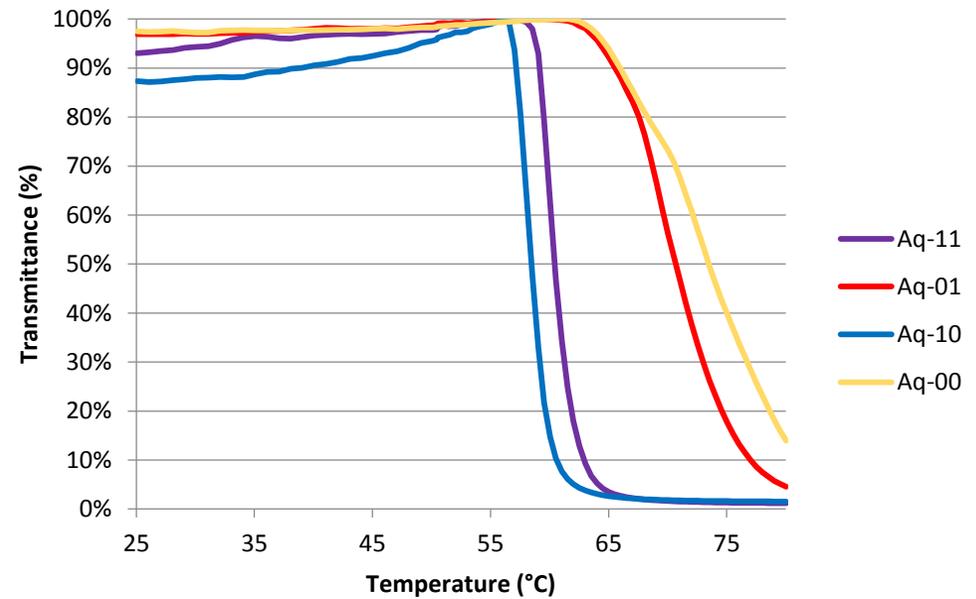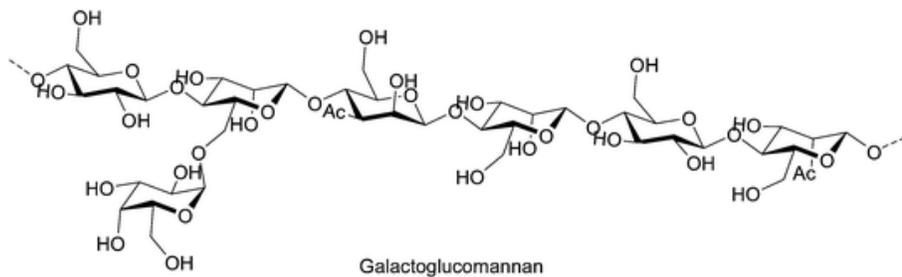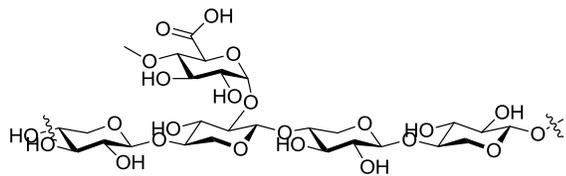
Questions

Detect small amount of specific atomic structure, molecular fragments

Assign how substituents are aligned on or out from particle surface

     In dilute water solution

     Interaction with matrix

If we have broad structure distribution (hemicellulose) what is possible to assign?

     Chemical structure, conformation, aggregation?

     under variable temperature, shear (rheology), pressure

Combine molecular modelling, prototypes with high resolution structure