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First and second order transition during water adsorption in hemicellulose and its consequence on hygro-mechanical behavior

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Arabinoglucuronoxylan (AGX) is one of the most abundant hemicellulose of softwood. It is formed by β-1,4-linked β-D-Xylp units, partially substituted at O-2 by 4-O-Me-α-D-GlcpA and at O-3 by α-L-Araf. It has diverse potential use in many industries, such as packaging of cosmetic or pharmacy, plastic additive and bio-refinery.
Despite its versatile potential, most of the key properties of xylan remain mysterious as it is difficult to isolate this polymer from wood sources without chemically altering it. Hemicellulose interacts strongly with moisture and induces many physical or mechanical changes. In this study, we apply molecular dynamics to investigate the mechanism of moisture influence on AGX.
Moisture induces various changes to AGX, such as isotropic swelling, enhancing diffusion, shifting pore size distribution, decreasing stiffness, etc. Besides the first order changes of properties upon moisture adsorption, there also exists a second order transition which means that properties considered as function of moisture develop two regimes separated by a transition zone. Water population distribution analysis shows that multi-layer adsorption is the mechanism of the second order transition. Moreover, we show that the main polymer of wood, e.g. amorphous cellulose (AC), does not show such second order transition as AC is more water miscible compared to AGX.

References

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