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Cellulose Nanofibrils Films: Molecular Diffusion through Elongated Sub-Nano Cavities

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Packaging technology is currently based on the use of petroleum-derived polymer materials. Environmental concerns, production costs and end-of-life disposal challenges require the introduction of innovative packaging materials produced using green technologies and able to meet requirements such as biodegradability and carbon neutrality. Cellulose nanofibrils (CNF) are highly stable nanostructures obtained from cellulose pulp that show excellent optical and mechanical properties. CNF films and CNF surface coatings attract great technological interest in order to replace the petroleum-based commercial packaging materials. Gas-phase permeation measurements show that few nanometers thick CNF films are impermeable barriers for CO₂, O₂, and N₂ but permit the selective transport of 2H₂ and He. Diffusive paths consist of interconnected elongated cavities between tightly packed cellulose nanofibrils. Depth-profiled positron annihilation lifetime spectroscopy measurements in the 1–12 keV positron implantation energy range with the pulsed low energy positron beam (PLEPS) at the MLZ in Garching indicate a cavity size of ~0.31nm, suggesting that the selective transport of small penetrants is due to sieving effects. Diffusion has configurational character and occurs by thermally activated process with 39 ± 1 and 33 ± 2 kJ mol⁻¹ activation energy for 2H₂ and He, respectively. Roilo et al., J. Phys. Chem. C 121 (2017) 15437–15447, DOI:10.1021/acs.jpcc.7b02895

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