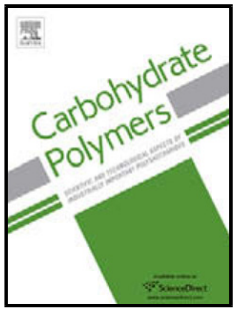

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Understanding the mechanisms of oxygen diffusion through surface functionalized nanocellulose films

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Highlights

- CNF films with low oxygen permeability at high humidity was achieved.
- Continuous nanometer-range layer is crucial for low oxygen permeability.
- Oxygen diffusion through film is govern by interactions with both oxygen and water.

Abstract

A concept for direct surface modification on self-standing films of cellulose nanofibrils (CNF) is demonstrated using an aminosilane group in cellulose compatible solvent (dimethyl acetamide, DMA). The chemically modified structure efficiently prevents the oxygen molecules from interacting with the nanocellulose film in the presence of water molecules. Oxygen permeability values lower than 1 mL mm m^{-2} day^{-1} atm^{-1} were achieved at extremely high levels of relative humidity (RH95%). The aminosilane reaction is compared to conventional hydrophobization reaction using hexamethyldisilazane. The differences with respect to interactions between cellulosic nanofibrils, water and oxygen molecules taking place with aminated and silylated CNF films correlated with the degree of surface substitution, surface hydrophilicity and permeability of the formed layer. The self-condensation reactions taking place on the film surface during aminosilane-mediated bonding was decisive for low oxygen permeability. Experimental evidence on the importance of interfacial processes that hinder the water-cellulose interactions while keeping film's low affinity towards oxygen is demonstrated.

Keywords: Cellulose nanofibrils, CNF film, surface functionalization, aminosilane reaction, oxygen permeability, relative humidity

Chemical compounds: (3-aminopropyl)-trimethoxysilan PubChem CID 83756, Hexamethyldisilazan PubChem CID 13838,