

# Chemical functionalization of cellulose nanocrystals for photovoltaic applications



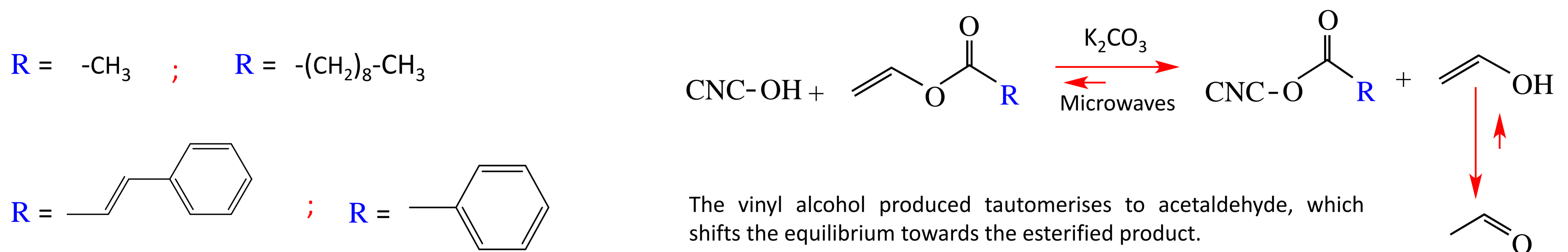
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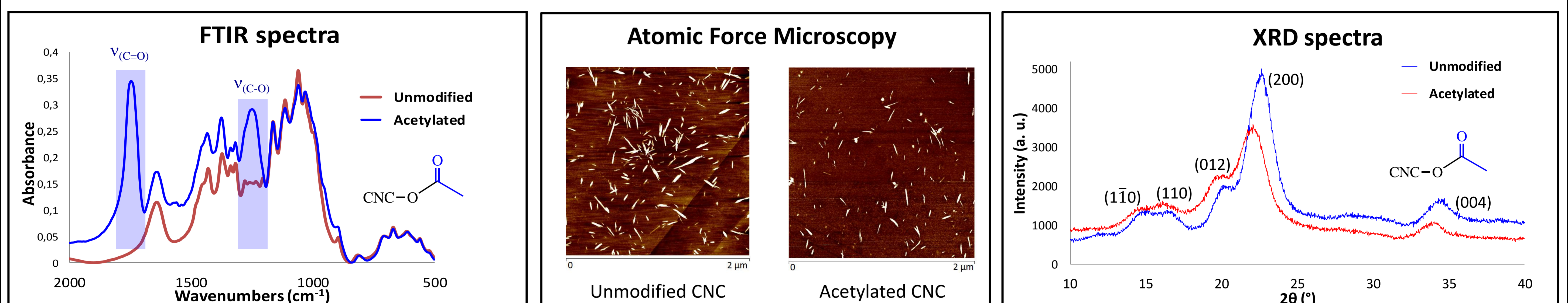


In this study, we envisaged tailoring the surface of cellulose nanocrystals (CNC) by chemical functionalization, in order to produce novel nanocomposite coatings for photovoltaic applications. An original functionalization method based on transesterification of vinyl esters is proposed (Sèbe et al. 2013, Jebrane et al. 2008) and applied to development of novel CNC-based coatings for solar cells, with improved mechanical and barrier performances.

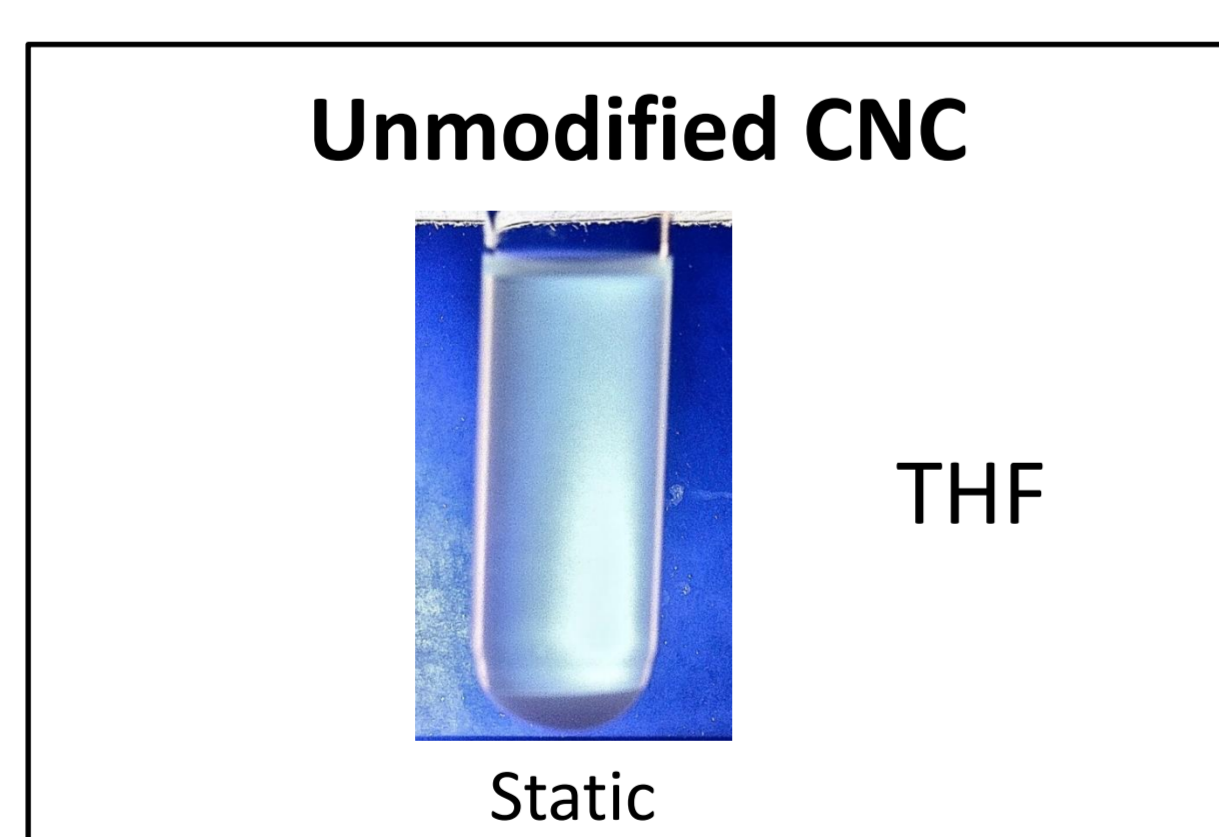
Esterified CNC can be obtained under mild conditions, with different vinyl esters as reactants:



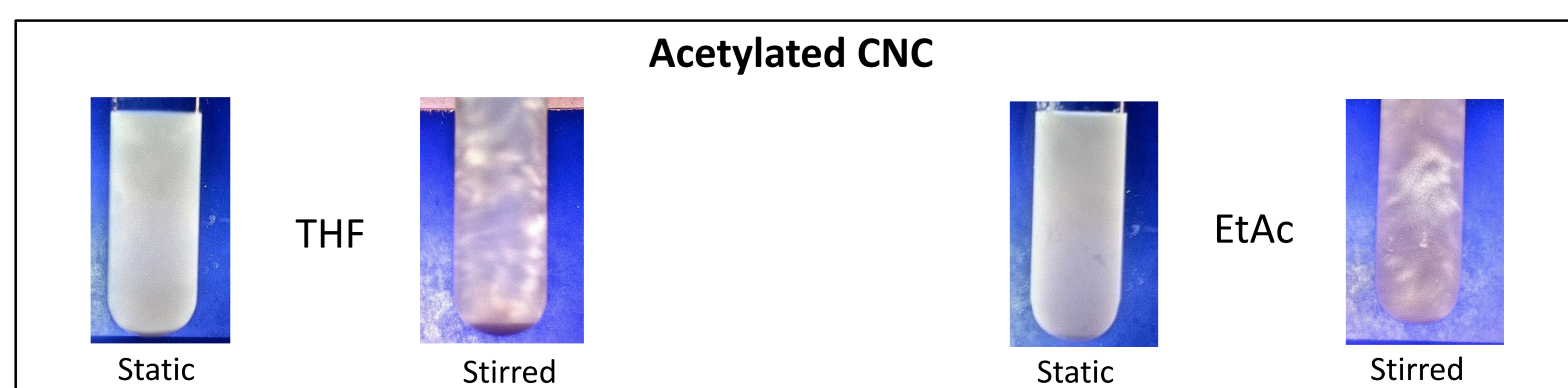
The grafting was confirmed by FTIR analysis, while the morphology and crystallinity were controlled by AFM microscopy and XRD spectroscopy, respectively. Highly substituted rod-like particles were obtained, with a limited loss in crystallinity:



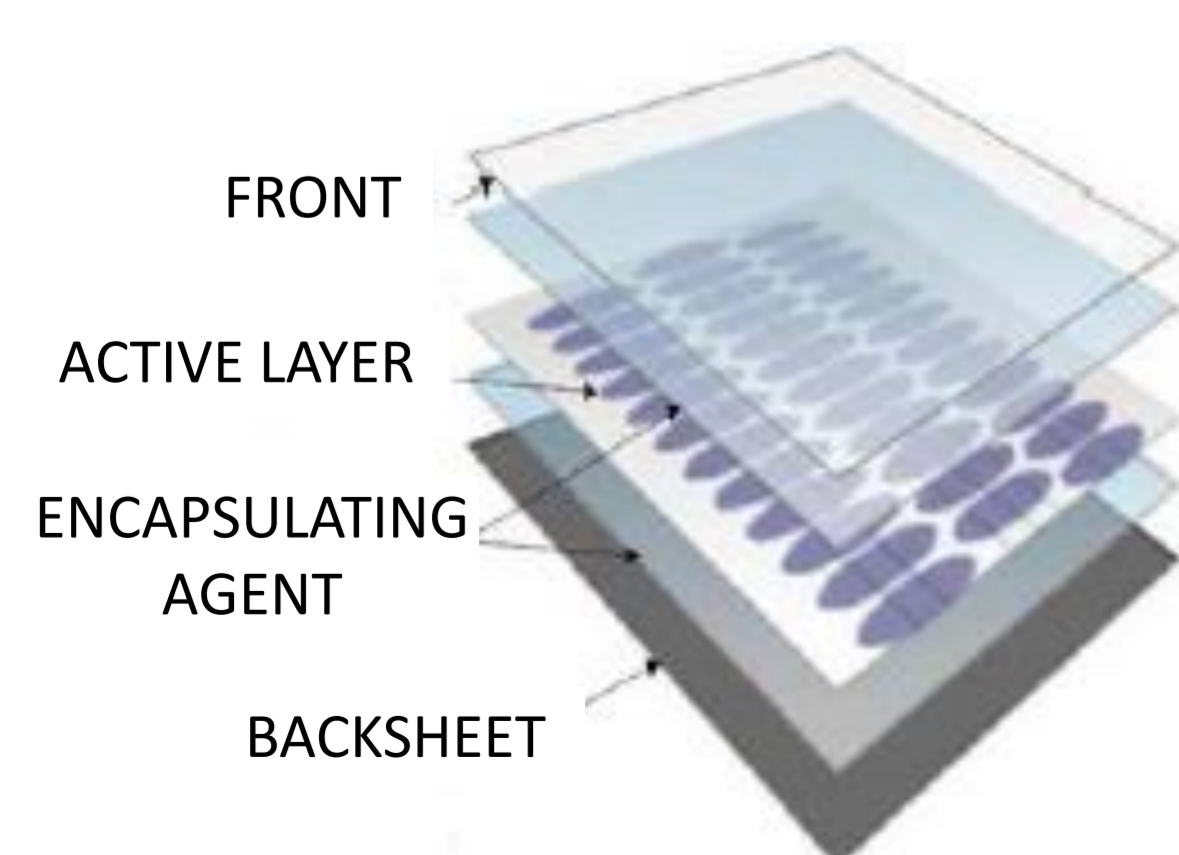
CNC are highly hydrophilic and can be dispersed only in polar solvents such as water ( $H_2O$ ,  $\epsilon = 80$ ), dimethylsulfoxide (DMSO,  $\epsilon = 46,7$ ) or dimethylformamide (DMF,  $\epsilon = 38$ ). After acetylation, stable dispersions were obtained in solvents of low polarity such as ethyl acetate (EtAc,  $\epsilon = 6,0$ ) or tetrahydrofuran (THF,  $\epsilon = 7,5$ ). The suspensions displayed flow-induced birefringence when observed between cross polarizers.



Flocculation



Stable dispersions (observation between cross-polarizers)



In future investigations, the esterified CNC will be applied to the elaboration of CNC-based coatings designed for solar cell, with the objective to improve the mechanical and barrier performances of the films.

The interfacial properties in the composite films will be monitored by controlling the chemical nature of the grafted function and the degree of substitution at the surface. The esterified CNC are also expected to increase the tortuosity of the diffusion pathway within the composite, which may lead to improved barrier properties against oxygen and water.

