

# Polymer nanocomposites with cellulose nanocrystals functionalised with 2-ureido-4[1H]pyrimidinone

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Cellulose nanocrystals (CNCs) are mechanically rigid, toxicologically benign, fiber-like nanoparticles, which can easily be extracted from renewable bio-sources and have attracted significant interest as a reinforcing filler in industrially produced polymers [1]. The polar nature of CNCs makes it however difficult to compound these particles with nonpolar polymers; indeed the thermodynamic immiscibility promotes the formation of micro- or macro-phase separated mixtures, unless very particular processing approaches are employed to circumvent this problem [2]. Alternative solutions include the functionalization of CNCs with non-polar surface groups [3], or decorating them with compatibilizing surfactants or polymers [3]. However, neither of these methods is universal, usually the reinforcing capability is reduced, and additional and sometimes complex and non-scalable processing steps are required. We have explored the use of the 2-ureido-4[1H]pyrimidinone (UPy) motif as “universal” compatibilizer for CNCs. Indeed, we show that UPy-modified CNCs [4] can be readily dispersed in nonpolar (toluene) as well as polar (dimethyl formamide) solvents, on account of morphing interactions: in the former solvent, the UPy motifs appear to form intra-CNC dimers, and in this state the particles appear to be “hydrophobized” and well-dispersible in a nonpolar environment. By contrast, the UPy motifs appear to dissociate in DMF and promote dispersibility through interactions with this polar solvent. We have exploited this feature to integrate UPy-modified CNCs into various host polymers and report on the mechanical properties of these materials.

## References

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