Electronic Supplementary Information

Ex-ante Life Cycle Assessment of polymer nanocomposites using organo-modified Layered Double Hydroxides for potential application in agricultural films

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Characterization of LDH platelets

The XRD data of the LDH platelets is presented in Figure 1. Their chemical compositions are given in Table 1. The XRD analyses of the hybrid LDH and polymer nanocomposites were performed on a Siemens D501 diffractometer using a Cu Kα source (30 mA, 35 kV); data were collected in a step scan mode between 2.0 and 70.0°(2θ) and with a step size of 0.03°(2θ) and a counting time of 10 s/step).

Surfactant-type anions are organized in a layered structure as demonstrated by the numerous harmonic diffraction lines of small full width at half maximum (FWHM), indicating large coherence domains. The diffraction lines are progressively shifted towards smaller 2θ values from Zn_2Al-CO_3, Zn_2Al-P-HCA, Zn_2Al-DDS, to Zn_2Al-C18 (stearate) corresponding to the different sizes of the guest molecules, as CO_3 < P-HCA < DDS (C12) < C18. The resulting hybrid organic-inorganic LDH materials exhibit a layered structure well organized with the presence of pronounced basal reflections up to the seventh to tenth order. The reflections at low 2θ values are depicted by enlarging the corresponding angular domain (left graph of Figure 1). Additionally the observed reflection at 2θ close to 61° is consistent with the formation of a LDH phase, and associated to *(110)* diffraction reflection, this in the rhombohedral symmetry adopting the space group R-3m to describe the LDH structure. The position of the diffraction line *(110)* is constant at d = 0.152 nm regardless of the alkyl chain length or of the presence of CO_3 and P-HCA, as indicated by a dashed line in Figure 1. This leads to a cell parameter ***c*** of 0.304 nm in agreement with a metal ratio Zn to Al of 2.[1]

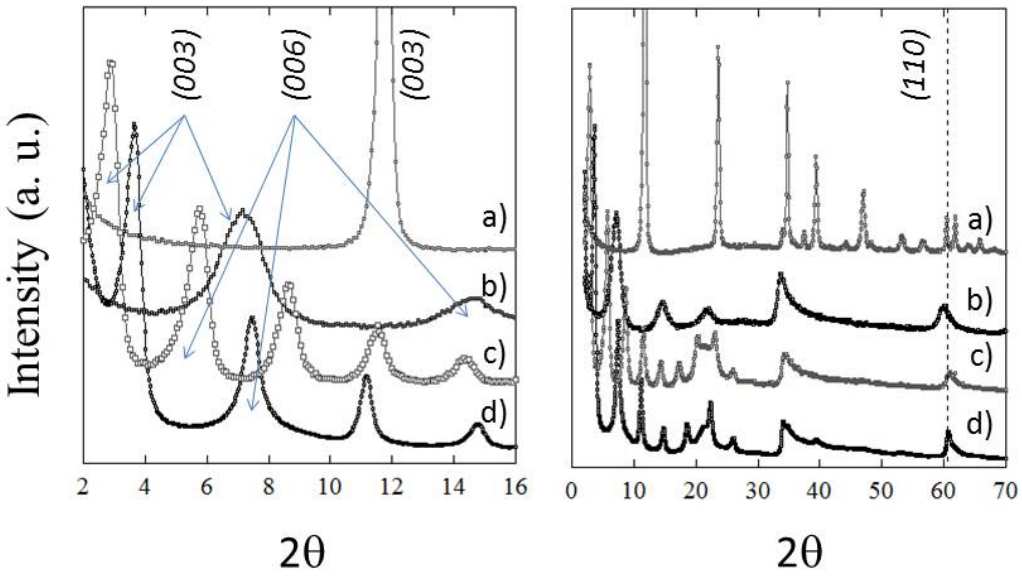

Figure 1 Typical XRD pattern of a) Zn_2Al-CO_3, b) Zn_2Al-P-HCA, c) Zn_2Al-DDS, and d) Zn_2Al-C18. The harmonic peaks (003) *and* (006) *are indicated as well as the Bragg diffraction peak* (110) *characteristic of the intralayer cation accommodation (see text) (P-HCA = p-hydroxycinnamic acid, DDS = dodecyl sulphate, C18 = stearate)*

Table 1 Chemical composition and basal spacing of the LDH (Zn-based) materials. Zn_2Al-CO_3 is included for comparison.

	Chemical composition	Basal spacing (nm)
Zn_2Al-CO_3	$Zn_{0.66}Al_{0.33}(OH)_2(CO_3)_{0.5}$ 1.5 H_2O	0.753
Zn_2Al-P-HCA	$Zn_{0.66}Al_{0.33}(OH)_2$(P-HCA)$_{0.98}$ 1.2 H_2O	1.228
Zn_2Al-DDS (C12)	$Zn_{0.66}Al_{0.33}(OH)_2(C12)_{0.99}$ 0.6 H_2O	2.402
Zn_2Al-C18	$Zn_{0.66}Al_{0.33}(OH)_2(C18)_{0.99}$ 0.4 H_2O	3.046

Intercalated anions are: P-HCA = $OH\text{-}C_6H_4\text{-}CH{=}CH\text{-}COO^-$; C12 = $C_{12}H_{25}OSO_3^-$; C18 = $C_{18}H_{35}O_2^-$

References

1. M. Hennous, Z. Derriche, E. Privas, P. Navard, V. Verney, and F. Leroux, *Appl. Clay Sci.*, 2013, **71**, 42–48.