Structure and dynamics of Lactose/ Montmorillonite Nanocomposites

MICHAEL HOLMBOE[1*], JOEL HELLRUP[2], DENNY MAHLIN[2]

[1]Department of Chemistry, Umeå University, Sweden (*correspondance to michael.holmboe@umu.se)
[2]Department of Pharmacy, Uppsala University, Sweden

Understanding how water sorption and moisture affect environmental and industrial product surfaces is essential for predicting their overall interfacial chemistry. For multicomponent composite materials the sorption behavior and surface properties are not always easy to predict based on the properties of the pure components.

In this study we have investigated water sorption onto lactose/montmorillonite nanocomposites (Figure 1). Lactose is one of the most commonly used excipients in pharmaceutical drug delivery, food technology, flavoring and a simple hydrocarbon analogue which is highly hygroscopic in its amorphous form.[1] We report from a detailed structural investigation using powder X-ray diffraction and water adsorption isotherms experiments as well as molecular dynamics (MD) simulations followed by 1D mixed layer modelling (MLM).[2]

In conclusion, the lactose was intercalated in the Na^+-montmorillonite (MMT) interlayer space regardless of the clay content, drying rate, or humidity exposure. By calculating the X-ray layer transforms (G^2) for the lactose/MMT composites from MD, the lactose loading into the MMT interlayers was estimated by 1D-MLM. Furthermore, the decreased hygroscopicity of the composite material compared to the pure components was explained by the competition between the lactose hydroxyls and water molecules for the interlayer Na^+ counterions in the MMT interlayer space of the lactose/Na-MMT nano-composites.

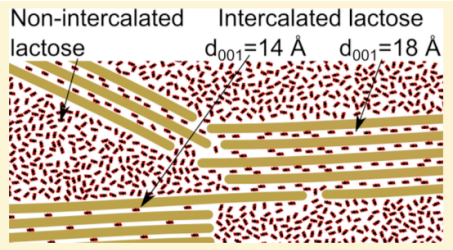

Figure 1. Illustration of the lactose/MMT composite particles showing Lactose intercalated as mono- or bilayered, resulting in basal spacings of 14Å and 18Å, resp.

[1] Hellrup, J., et al., Langmuir, **32,** 13214-13225, (2016).
[2] Ferrage et al., Clay Clay Min, **64**(4),346-371, (2016)