Understanding the barrier properties of dry, clay-based coatings. A contribution from computational modelling

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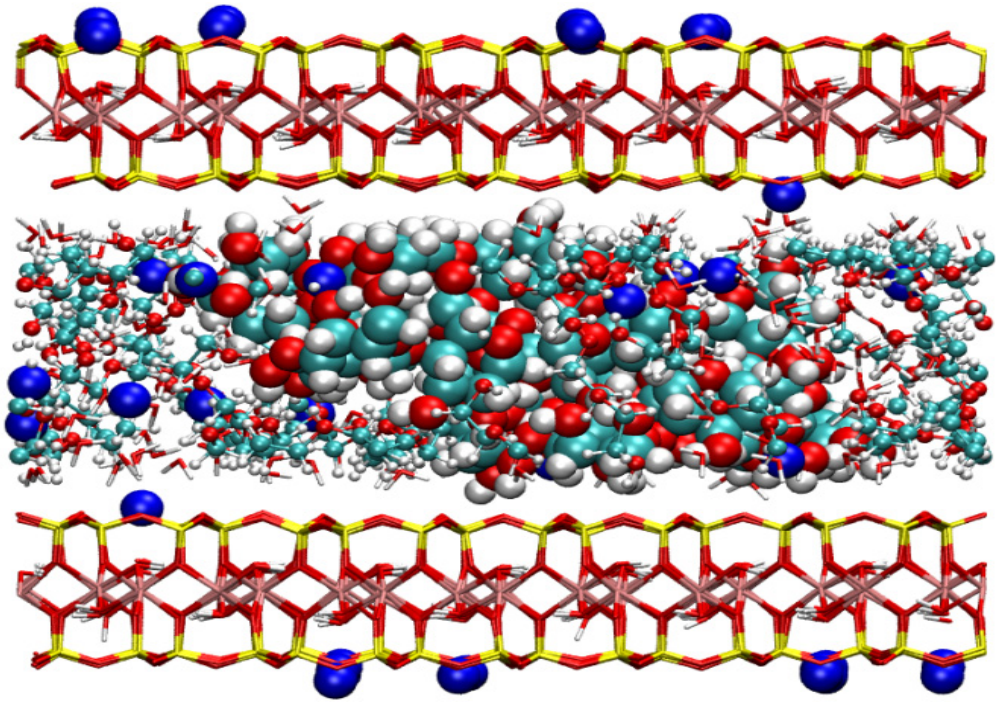
Coatings with high barriers to gases, vapours and flavours find their major application in food packaging materials[1]. Taking into account the amount of food currently wasted every year, packaging that keeps it fresh for a longer time has an important role to play in reducing the amount of energy consumed during the food production and transport cycle. Moreover, the importance of using sustainable packaging materials has become apparent over recent decades. This can be achieved by replacing the petroleum-derived additives (e.g. plastics) used when coating paper and board packaging by greener alternatives that still deliver the barrier and other crucial properties needed for competitive, low carbon footprint packaging materials.



Driven by this inspiration, a recent experimental study[1] has demonstrated that naturally occurring swelling clay minerals (in particular the smectites) can when combined with starch and bio-based plasticisers, provide sustainable paper coatings which are competitive with oil-derived barrier coatings. Experimental characterization of the molecular-scale structure and dynamics within the interlayer space in these systems gives little information due to static and dynamic disorder. It can, however, be obtained via use of molecular dynamics (MD) simulation techniques based on classical force fields[2].

To extend understanding of the roles played by clay, water and bio-polymers in these sustainable coatings and their respective impact on the resultant barrier properties, we have initially employed MD simulation to validate our models using experimental observations. Subsequently, the influence of clay charge location, cation exchange capacity, and interlayer cation on the equilibrated interlamellar arrangement in the clay-polymer composite was derived from the simulation study.With the combination of the results of the two methods, we can provide new insights for understanding the sorptive characteristics of the polymer-clay composites studied.

Current work is supported by European project NewGenPak (Marie Curie International Training Network (ITN), FP-7-PEOPLE-2011, project number 290098)

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