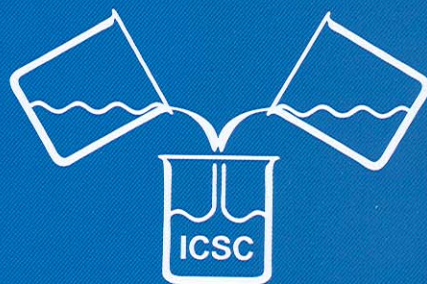


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## Simulation Insights on the Structure and Energetics of Biocompatible Polymer Nanocomposite Systems

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The structural arrangement and dynamical behavior of H<sub>2</sub>O molecules, ions, and other molecular species in the confined spaces of nano-scale pores and mineral interlayers are key to understanding transport and reactivity in many technological and biological systems. In this respect, considerable research efforts have been focused on the design of nanoscale oral sustained- and controlled-release drug delivery systems.<sup>1</sup> Special attention has been given to finding a way to regulate the rate of drug release by means of monolithic devices where the drug is dispersed or included in an inert matrix.<sup>2,3</sup> A way to produce inclusion compounds with drugs is given by their intercalation in a lamellar host lattice. Recently, for instance, it has been shown<sup>4</sup> that Mg-Al-hydrotalcite (HTlc), an inorganic and biocompatible anionic layered solid, can intercalate two well-known non-steroidal anti-inflammatory drugs (NSAIDs) such as ibuprofen and diclofenac, and modify their release. In order to couple these features with enhanced mechanical properties in systems to be exploited, for instance, as degradable polymeric implants that can also be used simultaneously to deliver therapeutic drugs to treat infections, polymer clay nanocomposite loaded with NSAIDs can be designed.

Based on our experience in the field,<sup>5-7</sup> in this work we present the results obtained from the employment of atomistic computer modeling to investigate the structure, morphology, and energetics of two different polymer nanocomposite systems based on the two NSAIDs ibuprofen and diclofenac, hydrotalcite and two different biocompatible polymers, poly( $\alpha$ -hydroxybutyrate) and poly(vinyl alcohol).

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