Molecular Dynamics Simulation Study on the Interfacial Interactions in Polyethylene-Organoclay Nanocomposites

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Polymer/clay nanocomposites has emerged as a new class of materials due to their increased mechanical, thermal, gas-barrier, inflammability properties. Prior to addition of polymer, surface modification of hydrophilic clays is needed by ion exchange reactions of organophilic cations for sodium ions to achieve good interfacial adhesion. These cations are alkyl ammonium chains also expand the layer or basal spacing; and the increased spacing helps polymer chains to form intercalated and exfoliated nanocomposites. For a highly nonpolar polyethylene, the interaction between the hydrophopic polyethylene and relatively hydrophilic organomodified clay surface is not as strong as desired. To overcome this limitation, some functionalized polyethylenes are used as a compatibilizers to increase their polarity and interactions with the organoclay. The success of nanocomposite depends on how clay layers are exfoliated in the polymer matrix. In this study, different Na-montmorillonite clays models are optimized by plane wave (PW) density functional methods (DFT). Nanocomposite structure and its properties are determined by using molecular dynamics (MD) simulation technique. Effect of alkyl ammonium chain lengths on the interlayer interactions and basal spacing are analyzed. The most stable positions of polar alkyl ammonium heads on the clay surface are found. The most effective interaction between the organoclay and different compatibilizers are sought.

References: