From Micro to Macroscale Theoretical Study for Polyethylene-Organoclay Nanocomposites

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Polymer-clay nanocomposites offer a wide range of enhanced properties arising from the reinforcement of clay nanoparticles in the polymer matrix. Further development of polymer-clay nanocomposites depends on the understanding of the micro and macro structures. This makes computational chemists to search new modeling and simulation strategies to provide a procedure which bridges the atomistic and mesoscopic simulations [1]. By this way, it is possible to explain the hierarchical characteristics of the structure and dynamics of polymer nanocomposites ranging from molecular scale, microscale to mesoscale [2].

In this study, polyethylene-organoclay nanocomposites are modelled by a series of hierarchical computational methods are linked in such a way that the calculated properties from a computational simulation at one scale are used to define the parameters of the model operative on the adjoining larger scale. Such parameter-passing, sequential approaches have proven to be effective, especially when material have components with several scales, each with different characteristics [3].

Montmorillonite clays with different cation exchange capacity, polyethylene oligomers functionalized by itaconic acid, maleic anhydride and acrylic acid groups and alkylammonium groups with different alkyl lengths and head groups were modelled and optimized by using Density Functional Theory methods in DMOL3 software installed in Materials Studio 4.0[4]. Atomic charges and optimized structures were needed for the molecular dynamics simulation methods which are used to understand dynamics and formation of nanocomposites, in addition to the interaction energies between the components of nanocomposite. The next step is the mesoscale simulations that is achieved by mapping the corresponding energy values and structures obtained from MD simulations to the interaction parameters and structures of the mesoscopic model.

The effect of grafting and grafting ratio, alkyl ammonium chain length and head groups, clay layer atomic charges on the nanocomposite properties are investigated in different range of time and length scales.

References:
[4]. Materials Studio 4.0, Accelrys, San Diego.