Computer simulation of polypropylene/organoclay nanocomposites: characterization of atomic scale structure and prediction of the binding energy.

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Molecular mechanics/dynamics computer simulations are used to explore and characterize the atomic scale structure, and also to predict binding energies of polymer/clay nanocomposites based on polymer (polypropylene and maleated polypropylene), montmorillonite (MMT) and several different alkylamonnium ions as surfactants. For each selected ammonium ions (quats), a molecular dynamics simulations were performed at 300-600 K for 100-300 ps with time step of 0.001 ps on computer model built from polypropylene (or maleated polypropylene, considered in the modeled 15 monomer units), montmorillonite platelet and 5 quat molecules. Several conformations were selected from the equilibrated time region, energy minimization carried out, and binding energies were calculated between individual components of nanocomposite. This model is performed with the prediction of uniformly dispersed platelets within polymer matrix.
Defoliation process was also modeled showing the importance of surfactant molecules. The modeling also enabled to design the structural modifications of polymer and surfactant to improve the properties of nanocomposites.