Computer simulation of polymer-organoclay nanocomposites for packaging applications: from binding energy to interlayer spacing predictions

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In recent years, organic-inorganic nanoscale composites have attracted great interest since they frequently exhibit unexpected hybrid properties synergistically deriving from two components. One of the most promising composite systems is the hybrids based on organic polymers and inorganic clay minerals consisting of layered silicates. Compared to their micro and macro counterparts, and the pristine polymer matrix, polymer clay nanocomposites (PCNs) can exhibit many advantages, including the following: a) they are lighter in weight than conventionally filled polymers because high degree of stiffness and strength are realized with far less high-density inorganic material, b) they exhibit outstanding diffusional barrier properties without requiring a multipolymer-layered design, c) their mechanical properties are potentially superior to unidirectional fiber-reinforced polymers, because reinforcement from the inorganic layers will occur in two dimensions rather than in one, and d) improved solvent and UV resistance, greater dimensional stability, and superior flame retardancy.
In this work, molecular mechanics/dynamics computer simulations are used to explore the atomic scale structure and to predict binding energy values and d-spacing for polymer/clay nanocomposites based on two different polyamides (nylon-6 and ADS 40T), montmorillonite and several, different quaternary ammonium salts.