Computer–aided based technology in polymer silicate nanocomposites: a new approach for fast screening of good surfactants based on atomistic and mesoscale molecular simulations

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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 (PCNs).

Similarly to polymer blends, any mixture of a polymer and layered silicate does not necessarily lead to a nanocomposite. In most, the incompatibility of the hydrophilic nature of the silicates and the hydrophobic character of most engineering polymers will induce a phase separation, similar to that of macroscopically filled systems. Therefore, the selection of a suitable surfactant, which contributes to render the clays organophilic and to lower the surface energy of the clay layers, becomes a prominent issue in PCN design.

The interactions between polymer and surfactant play a major role in promoting the intercalation of the macromolecules within the galleys of the pre-treated nanofiller. Indeed, the formation and the equilibrium structure of a organically modified polymer layered silicate nanocomposite is a strong function of the nature of the polymer as well as the chain length and structure of the surfactant.

The aim of this work is twofold: a) the development of a methodology to determine the suitable mesoscale parameters for a given polymer-surfactant couple and b) the use of mesoscale simulations to rank the surfactant molecules by increasing efficiency on the basis of the segragation level of the resulting morphology.