

How good a surfactant for polymer silicate nanocomposites can be? Answers from atomistic and mesoscale molecular simulations

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The in situ formation and assembly of silicate nanoparticles with high aspect ratio represent the key to novel structural and functional polymeric materials with skeleton-like silicate superstructures. One of the most promising composite systems is the hybrids based on organic polymers and inorganic clay minerals consisting of layered silicates (PCNs).

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 an organically modified PCN 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 segregation level of the resulting morphology.