Warwick Centre for Predictive Modelling Seminar Series

Computational modelling for performance improvement of polymer nanocomposites

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R0.12, Ramphal Building, Ground Floor

Abstract: Development of novel multifunctional polymeric nanomaterials such as polymer nanocomposites requires a careful control of nanoparticle dispersion and distribution in a polymer, and a thorough understanding of polymer-nanoparticle interactions. Multiscale computational models can provide insight into the effects of material composition (e.g. nanoparticle functionalization) and process conditions (e.g. temperature), on the evolution of nanocomposite morphology during processing, and thus on nanocomposite end-use properties (e.g. mechanical).

This presentation will give an overview of a computational modelling methodology to predict the processing and properties of the nanocomposites. It will be illustrated with some computational examples, such as those related to secondary processing of organo-nanoclay-based thermoplastics near the glass transition, and a nonlinear rate-dependent mechanical response of thermoset-CNT systems.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars