

Facets of Materials Modelling at Henkel

Marc Hamm

Henkel AG & Co. KGaA, Düsseldorf

Simulations and modelling are an evolving discipline in the development of products and materials, which Henkel brings to market. These include adhesives as well as laundry and beauty-care products. The customer demands do structure the type of models which are applied. Here the main factor determining the modelling approach is the time scale of customer expectation. The scope of these approaches will be presented ranging from statistical models, over finite elements, dissipative particle dynamics, molecular mechanics, to density functional theory. The presentation of these models will be completed by a discussion of what makes business sense.