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Using Modeling to Design new Rheology Modifiers for Paints[1]

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Since their invention in 1970-s, hydrophobically ethoxylated urethanes (HEUR) have been actively used as rheology modifiers for paints. Thermodynamic and rheological behavior of HEUR molecules in aqueous solutions is now very well understood and is based on the concept of transient network (TN), where the association of hydrophobic groups into networks of flower micelles causes viscosity to increase dramatically as function of polymer concentration. The behavior of complex mixtures containing water, HEUR, and latex ("binder") particles, however, is understood less well, even though it has utmost importance in the paint formulation design. In this talk, we discuss how the adsorption of HEUR chains onto latex particles results in formation of complex viscoelastic networks with temporary bridges between particles. We then utilize Self-Consistent Field Theory (SCFT) model to compute effective adsorption isotherms (thickener-on-latex) and develop a rheological theory describing steady-shear viscosity of such mixtures. The model is able to qualitatively describe many important features of the water/latex/HEUR mixtures, such as strong shear thinning. The proposed approach could potentially lead to the design of new HEUR structures with improved rheological performance.

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