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(G*) Dispersion and Orientation Patterns in Nanorod-infused Polymer Melts

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The dispersion and orientation of nanorods in a polymeric matrix have a direct impact on the mechanical and physical properties of the final material. Our molecular dynamics simulations show a direct relationship between the concentration and the order of the system when rod-polymer attractive interactions are applied. At lower concentrations, nematic droplets of nanorods form while at higher concentrations, the nanorods distribute isotropically and uniformly throughout the melt. This behaviour is attributed to the interplay of the enthalpic and entropic effects. A closer look at the conformation of the polymers also reveals that the interfacial chains are stretched out and have higher radius of gyrations.

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