Using Molecular Dynamics Simulations to Study the Self-Assembly of Patchy Alkane-Tethered Nanoparticles

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The addition of nanoparticles to materials has the ability to enhance a variety of characteristics such as their mechanical and optical properties. These properties are often highly correlated with the arrangement of nanoparticles within the material. Self-assembly of nanoparticles into structures can be controlled by modifying their surface properties: for example, by attaching organic chains with different terminal groups to parts of the nanoparticle surface. One route to guiding self-assembly can be achieved through the use of “patchy” nanoparticles, i.e. nanoparticles with partial coatings; however, in this work, the “patch” is not the exposed nanoparticle core but instead another type of chain with dissimilar chemical properties. This results in a completely coated nanoparticle. In this work, coarse-grained molecular dynamics simulations are used to examine self-assembly of patchy nanoparticles. We examine nanoparticles featuring several anisotropic polymeric coating patterns with two or more chain types, such as an equatorial pattern where a second chain type is placed as a band around the equator. Adjustable properties include the fractional surface area of each chain type, the strength of interactions between chain types, chain lengths, and coating density measured in attached chains per nanometer squared of the surface. Previously, we found that these properties can be used to encourage nanoparticle self-assembly into a variety of phases, including dispersed, strand-like, and aggregate phases. This continues to be true with more complex coating patterns, especially patterns that can form two-dimensional structures. The results of this work enhance knowledge of the phase space of patchy nanoparticles and will aid in the design of better performing materials.

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