Graphene Sheets-Oil Nanocomposites: Equilibrium and Transport Properties from Molecular Simulation

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Nanostructured materials hold unrestricted promise in catalysis, material science and engineering. It has long been thought that dispersing nanoparticles in a polymer blend can enhance both mechanical and transport properties. It would be, for example, desirable to generate a polymer nanocomposite with high thermal conductivity. Such materials could be obtained by dispersing thermally conductive nanoparticles within polymers. Carbon-based nanoparticles are extremely promising towards these goals, although the use of carbon nanotubes is hindered by high resistance to heat transfer from the nanotubes to the polymer matrix.

We are interested in composites in which graphene sheets (GS) are dispersed within organic oils. We observed that pristine GS agglomerates when dispersed in oils such as octane, hexane and dodecane. However, our equilibrium molecular dynamics simulations demonstrate that when the GS are functionalized on their edges with short-branched hydrocarbons, they remain well dispersed within the oils for up to 100 ns. Because our goal is to control the composite thermal transport by manipulating GS self-assembly, we are conducting equilibrium and non-equilibrium molecular dynamics simulations to assess the effective interactions between GS dispersed in oils, the self-assembly of GS within oils, the structure of the fluid surrounding the GS, and the heat transfer from a GS to the surrounding matrix. Our tools are designed to understand the effect of GS size, oils' molecular weight and molecular architecture on the GS dispersability and GS-oil heat transfer rate. We will discuss our results and how they could be used to design novel polymer nanocomposites.