

Problem Definition:

Matrix-free polymers grafted with nanoparticles (ex. cellulose nanocrystal, gold, silicon dioxide, etc.), commonly known as assembled hairy nanoparticle (aHNP), shows significant alteration in mechanical properties, such as modulus, strength, toughness. The increased structural order due to added nanoparticles helps to tailor its properties for specific applications. The enhancement strongly depends on the various design parameters like grafting density, polymer chain length, polymer chemistry, nanoparticle radius, side-chain group, etc. For example, the fracture toughness of aHNP changes when the polymerization increases beyond a certain limit. The polymer conformation changes from concentrated brush regime (CPB) to semi-diluted brush regime (SDPB). So, it is essential to find out the right design parameters to optimize their properties. However, laboratory experiment on aHNP with different all design parameters is very exhaustive and practically impossible. A data-driven method is a right way to solve this problem.

Methodology:

The first step is to collect significant data by varying design parameters. For that, coarse-grained molecular dynamics simulations are used. In CG-MD, one monomer unit is modeled by one or two beads depending on the polymer type. This way, it reduces the computational cost and enables us to collect a lot of data quickly. The design parameters that can be varied are polymer chain length, grafting density, polymer-nanoparticle interaction and nanoparticle geometry. The next step is to find out important features. For aHNP, toughness and ultimate strength are two important mechanical parameters. Third step is dimension reduction. The initial study finds that strength and toughness depend strongly on chain length and grafting density. However, all four parameters are considered for later steps. Now the simulation data can be used to train a neural network which will use the design parameters as the inputs and the output from the model will be toughness and ultimate strength. After training and validation, the mechanical properties can be directly computed from the neural network without running any simulation. This will help us to explore the large design space very quickly and find out the optimized design parameters for desirable mechanical properties.