Homework 6
Polymer Physics 2024
Due Tuesday February 20 at noon
(**pdf** file should be called: HW 4 Group x Last Name_Name_Name_Name.pdf)

There has been interest in the production of single-chain nanoparticles (SCNPs) for about 10 years. These structures have been linked with naturally occurring native state proteins which are collapsed polymers. The process of protein folding is generally seen as progressing from a self-avoiding walk in a good solvent, collapse to a 3D molten globule, and finally rearrangement into a native state functional protein. Some proteins are functional in the unfolded state, natively unfolded proteins. Zhang L, Zhang XZ, Lyu JT, Yu LX, Wang CY, Sun ZY Lu ZY, Qian HJ, *Surface-Cross-linked Protein-like Single-Chain Nanoparticle Globules Unexpectedly Stabilized with a Low Cross-linking Degree* Macromolecules **57** 858-868 (2024) propose that a functional SCNP can be produced by polymerizing random copolymer chains with a small fraction of UV curable monomers that have solubility in a nonsolvent for the main chain so that the chains in dilute conditions in a non-solvent collapse with crosslinkable groups on the surface. Once these surface groups are exposed to UV a SCNP is formed. The SCNP has residual crosslinkable groups that can be used to react SCNPs forming a hierarchical structure.

a) Zhang demonstrates that curing the random copolymer in a good solvent increases the size of the chains, while curing the copolymer in a poor solvent for the major component results in smaller chains. Use Scheme 1 on page 859 to explain this observation.

b) Zhang uses dynamic light scattering which measures the mean square displacement of particles $<x^2>$ as a function of time? Explain how this can be used to obtain the hydrodynamic diameter in Figure 1b using the Einstein-Stokes equation. Derive the Einstein-Stokes equation as done in class.

c) Zhang reports the molecular weight from GPC measurements based on equivalent polystyrene molecular weights using an index of refraction detector. What does the molecular weight value actually reflect? If he had a more expensive GPC with a viscosity detector and a light scattering detector, how could he have improved on his conclusions?

d) In Figure 3, Zhang shows, from CGMD simulations, that the reactive groups are close together along the contour length position X in the non-solvent, and far apart in X for the non-solvent. Explain what the contour length is and why the position of the functional groups along the contour length in the final polymer makes a difference.

e) Figure 6 shows the good-solvent, self-avoiding chain as having a power-law decay of -1.7 slope in X-ray scattering. If you look closely at Figure 6a the slope is a little shallower than -1.7, closer to -5/3. Derive the origin of this slope by going through the Flory-Krigbaum derivation and explain how scattering can be used to verify this behavior.