

Project plan (the rest of it ...)

- 1) Test new code in pysoftk to see that it works for building
 - a. linear block co-polymers consisting of asymmetric monomers (use any combination of the previously stated asymmetric monomers)
 - i. Diblock
 - ii. Triblock
 - iii. Random two component
 - iv. Random three component
 - b. (when the code is available from Alejandro) cyclic polymers with symmetric and asymmetric monomers
 - i. Homopolymers
 - ii. Diblock
 - iii. Triblock
 - iv. Random two component
 - v. Random three component
 - c. (when the code is available from Alejandro) x-shaped polymers with symmetric and asymmetric monomers as arms
 - i. Homopolymers
 - ii. Diblock
 - iii. Triblock
 - iv. Random two component
 - v. Random three component
- 2) Create scripts (like those you previously generated) to build other novel topologies of polymers (these will then be used by Alejandro to create functions within the pysoftk code itself as has been done already for the asymmetric monomers and soon the x-shaped and cyclic polymers)
 - a. Bottle-brush
 - b. Star polymer
 - c. Miktoarm star polymer
 - d. Dendrimer
- 3) Make pictures that we can include in the paper which will be published (relatively) soon about the pysoftk code. This pictures should have a screen grab of the code used to generate a given set of monomers and then the polymer alongside pictures of the chemical structure of the monomers and polymer (as generated in pysoftk) and pictures of the molecular structure of the monomers and polymers (created with vmd). For some inspiration (at least for the code bit) please see the LiPyphilic paper (which is in the papers directory).

We would like pictures of

 - a) Linear symmetric polymers:
 - a. Homopolymer
 - b. Random heteropolymer
 - c. Diblock co-polymer
 - b) Linear asymmetric polymers:
 - a. Homopolymer
 - b. Diblock co-polymer
 - c) Ring asymmetric polymers:

- a. Homopolymer
 - b. Diblock co-polymer
 - d) X-shaped asymmetric polymers:
 - a. Homopolymer
 - b. Diblock co-polymer
- 4) Then I would like to give you the experience of running at least one molecular dynamics simulation so we can do that as well if you have time.