Structure Work

Polymers in Solution

Equilibrate Glycolated polymer in NPT.

Extract measured monomer X-ray patterns.

Characterise pi-stacking in the two structures.

Holiday

Continue trying to get monomer xrd patterns from chrysalis

Write second draft for abstract that I would have submitted to conferences

Have talks with Alex and Camilla about findings. Discuss what the implications might be for devices. Discuss how these effects might be tested.

More thorough characterisation of the MD simulations done so far. Include auto-correlation functions, 'F' parameters etc.

Characterise the herringbone structure obtained for glycolated polymer.

Look at alternate glycolated polymer structures which contain a pi-stack system.

Bank Holiday

Simulations of crystallites in solution to investigate solution diffusion into crystallites

Write bullet-point plan for a paper

**Simulations of single polymers in solution to investigate polymer-solution interaction.
Analysis of solution rdf etc shells etc.**

Familiarise myself with literature and write literature review for paper.

Simulate and characterise amorphous phase for polymers (include mixed side chains)

Develop structure paper and write

16th Mar | 23rd Mar | 30th Mar | 6th Apr | 13th Apr | 20th Apr | 27th Apr | 4th May | 11th May

Goals beyond this timeline -

- Simulations of micro-crystallites in solution to investigate the solvent effect on the crystal structure.
- Simulations of amorphous phase in solution to investigate the solvent effect on amorphous phase.
- Increase focus on dynamics. Are there interesting polymer-solvent interactions in terms of dynamics?
- PMF calculations of polymers in solution
- Develop forcefields for the p(g2T-TT) and p(a2T-TT) polymers, as well as those with the spacer units