Schedule: Self-Assembly Workshop

Thursday 22nd September

Todd-Hamied Room, Department of Chemistry

External Speakers

12:00	**12:30**	**Buffet lunch**
12:30	13:10	**Tim Totton** Kraft Group, Chemical Engineering, Cambridge
13:10	13:50	**Qibin Zhao** Baumberg Group, NanoPhotonics Centre, Physics, Cambridge
13:50	14:30	**Feng Tian** Scherman Group, Chemistry, Cambridge
14:30	**15:00**	**Tea and coffee**
15:00	15:40	**Chris Forman** Institute for Manufacturing, Cambridge (Barker Group, Chemistry)
15:40	16:20	**Anna Peacock** Chemistry, Birmingham
16:20	17:00	**Jonathan Bath** Turberfield Group, Physics, Oxford
18:00	20:00	**Dinner**

Friday 23rd September

Unilever Lecture Theatre, Department of Chemistry

General Instructive Talks, Progress Reports and Future Projects Discussion

		Short talks and progress reports:
9:30	9:50	Flavio Romano - GPU
9:50	10:10	Tom Ouldridge - DNA Walkers
10:10	10:30	Mark Miller - Website demonstration
10:30	**11:00**	**Tea and coffee**
11:00	12:30	Business Meeting

Afternoon for further discussions as required.

14:00 DNA discussion (JPKD and DF)

Tim Totton
Kraft Group, Chemical Engineering, Cambridge
Modelling soot formation with ab initio potentials

Polycyclic aromatic hydrocarbon (PAH) molecules are known precursor species in the formation of soot particles. To control soot formation we need to understand the underlying processes of PAH aggregation. Yet despite a lot of work in this field there remain several important unanswered questions: Is PAH aggregation by physisorption a feasible route to particle formation and growth at flame temperatures? If so, how large must a PAH be to make dimerisation possible in a flame? What are the rates of aggregation? How do inaccuracies in the intermolecular potentials affect findings? We approach this problem by developing accurate intermolecular potentials from ab initio SAPT(DFT) calculations. Using these we are able to accurately study the potential energy surfaces of PAH clusters and model the dynamic behaviour at flame temperatures, giving key insights into the soot formation process.

Qibin Zhao
Baumberg Group, NanoPhotonics Centre, Physics, Cambridge
Shear ordering in polymer opals

Polymer opals are soft 3D photonic crystals comprised of core-interlayer-shell polymer beads. By melting the shell and applying external force like compression or shearing, these spheres can be ordered into FCC lattice. Different from colloids, in which the solvent is independent and the viscosity is relatively low, the medium in polymer opals is attached to the core of the bead and highly viscoelastic, which gives some very interesting and unique behaviours under shearing.

Feng Tian
Scherman Group, Chemistry, Cambridge
Cucurbituril: At the Interface of Supramolecular Chemistry and Dynamic Self-Assembly

The remarkable guest binding behaviour of the synthetic receptors, cucurbit[n]uril, has gained tremendous attention over the past few decades. The stronger and more selective encapsulation of small guests has opened up the possibility to develop multi-component, dynamic yet controlled supramolecular aggregated architectures for a wide variety of applications. Isolation of larger homologues and derivatives have expanded the scope further, and interest has grown exponentially. Applications of these unique synthetic receptors presently range from polymeric smart materials and wet nanotechnology to sensing and protein conjugation. This talk highlights such examples from our recent work on the development of new dynamic supramolecular aggregates and composites using cucurbituril host-guest chemistry.

Chris Forman
Institute for Manufacturing, Cambridge (Barker Group, Chemistry)
Decorated Amyloid fibril morphology is controlled by the position and conformation of the displayed protein.

A range of fusion proteins, consisting of SH3 domains and electron transfer protein cytochrome b562, have been constructed which can self-assemble into amyloid fibres that display the cytochrome. The effect on fibre morphology of changing the position and conformation of the cytochrome is investigated experimentally using TEM, AFM, high resolution AFM and UV-Vis spectroscopy. These effects are quantified and then interpreted in terms of a simple model of bundles of filaments that interact mostly via the displayed cytochrome. To explore the validity of this model a minimal complexity coarse grain unit is developed which has been shown in silico to assemble into helical fibres. The morphology of the simulated fibres can be systematically altered by adjusting the parameters of the coarse grain unit that correspond to the introduction of non-core material in the fusion proteins. This useful new tool may help to design a fibre which is capable of mediating electron transfer along its entire length.

Anna Peacock
Chemistry, Birmingham
De novo peptide design: From metallopeptides to DNA binding proteins

De novo designed peptide constructs based on TRI, Ac-G(LKALEEK)4G-NH2, and CoilSer, form amphipathic α-helices in solution and above ca. pH 5 these aggregate to form three-stranded coiled coils. These scaffolds provide a stable framework in the interior of which we can design challenging metal binding sites by incorporating amino acids capable of binding to metal ions. Recently we have begun investigating binding of lanthanides to these coiled coils, and in particular are interested in exploring gadolinium coiled coils as novel MRI agents. Other projects investigate the DNA binding properties of synthetic peptides based on coiled coils containing a structural metal ion, as well as helix-loop-helix motifs, in which the α-helices are linked by 'artificial loops' capable of a measurable output.

Jonathan Bath
Turberfield Group, Physics, Oxford
Structures and devices built from DNA

DNA is an ideal construction material for self-assembled structures and devices. The strength and specificity of interactions between the component strands can be encoded in the nucleotide sequence. Assembly requires only that the component strands are mixed and annealed. I will describe the design and construction of free-running molecular motors where DNA is both construction material and fuel.