



# **Workshop on equilibrium and out-of-equilibrium molecular systems**

**ArtMoMa Summer School  
Simpkins Lee Room, Beecroft Building  
Department of Physics  
Parks Road, Oxford OX1 3PU  
25-26 July 2022 - Programme**

# DAY 1, Monday 25 July

## Research Lectures

10:15 - 10:45

Opening and registration

10:45 - 11:00

Welcome: Prof. Andrew Turberfield

11:00 - 12:00



**Functional Metallo-supramolecular Quadruplexes - Guido Clever, full Professor, TU Dortmund University, DE**

Research in the Clever Lab is motivated by fascination for the structural and functional complexity of nature's biochemical machinery. We work on the bottom-up design and construction of artificial devices, aggregates and complex systems on the nanometer scale, mainly based on (metallo) supramolecular chemistry.



12:00-13:30 - Lunch



13:30-14:30



**Templates for directing the synthesis of molecular nanorings and cages - Harry Anderson, Professor of Chemistry at the University of Oxford, UK**

My group has shown that oligo-pyridine templates can be used as construction tools to direct the synthesis of large covalent nanorings and cages, via coordination to metalloporphyrin components. This chemistry provides access to synthetic nanostructures in the size range of proteins with remarkable photophysical, electronic and magnetic properties.

# DAY 1, Monday 25 July

## Research Lectures

14:30-15:30



**Structurally Ordered Polymeric Materials via Dynamic Covalent Synthesis - Wei Zhang, Professor and Department Chair, Department of Chemistry, University of Colorado Boulder, US**

The Zhang group research is focused on the development of novel DCvC Reactions/catalysts and utilizing them to develop novel functional molecules and polymeric materials targeting a broad range of environmental, energy, and biological applications, such as carbon capture, molecular separation, nanocomposite fabrication, energy storage, and self-healing materials.

15:30 - 15:50



**Coffee Break**



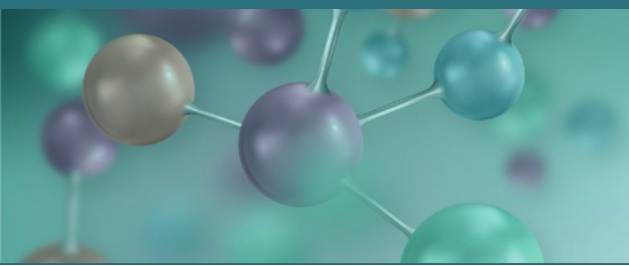
## **ArtMoMa EARLY STAGE RESEARCHERS**

15:50-16:30

**Flash presentations of individual projects**

16:30-18:00

**Poster session with refreshments**



# DAY 2 Tuesday 26 July

## Research Lectures

9:00-10:00



**Complex molecular topologies via reversible ring/loop threading - Makoto Fujita, University Distinguished Professor, The University of Tokyo (Zoom)**

Our group has introduced a new construction principle, featured as "metal-directed self-assembly", leading to the spontaneous formation of cyclic structures, catenanes, three-dimensional cages, and so on that are assembled from a large number of transition metal centers and simple coordinating organic molecules.

10:00-11:00



**The How and Why of Knotted Proteins, Sophie Jackson Professor of Chemical and Molecular Biology, University of Cambridge, UK**

For three decades after the first protein structure was solved, it was assumed that there were, and would be, no cases in which a protein chain tied itself into a knotted structure. In 2000, it was shown that knots, even deep knots, exist in a significant number of protein structures. The talk will briefly summarise what we have learnt about how proteins form knotted structures, and how the knots affect structure, stability, and function. The talk will finish with a section on recent designs of knotted proteins and what we have learnt from them.

11:00-11:30



**Coffee Break**



# DAY 2 Tuesday 26 July

## Research Lectures

11:30-12:30



**The synthesis and applications of mechanically chiral molecules - Steve Goldup, Professor of Chemistry, University of Southampton, UK**

We investigate the properties and applications of mechanically interlocked molecules, particularly chiral examples where the stereochemistry arises due to the mechanical bond. To achieve this, we also develop and optimise synthetic methods to access challenging structures so their applications can be studied.



12:30-14:00 Lunch



14:00-15:00



**Kinetic Asymmetry, the neglected ingredient in Chemical Coupling - Dean Astumian, Professor, Dept. of Physics and Astronomy, The University of Maine, US**

Chemical coupling plays the essential role in biological metabolism of providing a mechanism by which energy released in an exergonic chemical reaction can be used to drive a different chemical reaction energetically uphill. Through evolution, chemical coupling has come to be used also to drive the creation of concentration gradients across membranes via membrane molecular pumps and to harness chemical energy.

Recent work on synthetic molecular machines has reinvigorated efforts, both experimental and theoretical, to better understand chemical coupling.



# DAY 2 Tuesday 26 July

## Research Lectures

15:00-16:00



**Guest recognition in dynamic libraries and spin-crossover cages, Larissa von Krbek, Biochemistry, University of Bonn, DE**

Spin-crossover (SCO) metal-organic cages are capable of switching between high-spin and low-spin states, which enables these molecular containers to be used as magnetic sensors and switches. A SCO tetrahedral Fe(II) cage is capable of encapsulating various guests. Conversely, the SCO tetrahedron exhibits different affinities for the guests in different spin states, which is inferred to result from the subtle structural differences of the cavity caused by the change in metal centre spin state.

16:00-16:30



**Coffee Break**



16:30-17:30



**Origins of the RNA-Protein World - Lost in Translation? Professor John Sutherland, Programme Leader, MRC Laboratory of Molecular Biology, Cambridge UK**

In this lecture I will describe some mixed hydrogen cyanide-hydrogen sulfide chemistry that produces nucleotides and amino acids. Some degree of control is necessary for this 'cyanosulfidic' chemistry to proceed most efficiently and ways in which environmental factors could exercise this control will be suggested. Synergies in the assembly of nucleotide and amino acid building blocks into higher order structures will then be discussed. Finally it will be shown how the strength of codon-anticodon binding likely influenced the partial initial assignment of the primary genetic code.

**19:00 - 21:00 - Closing dinner, Magdalen College**