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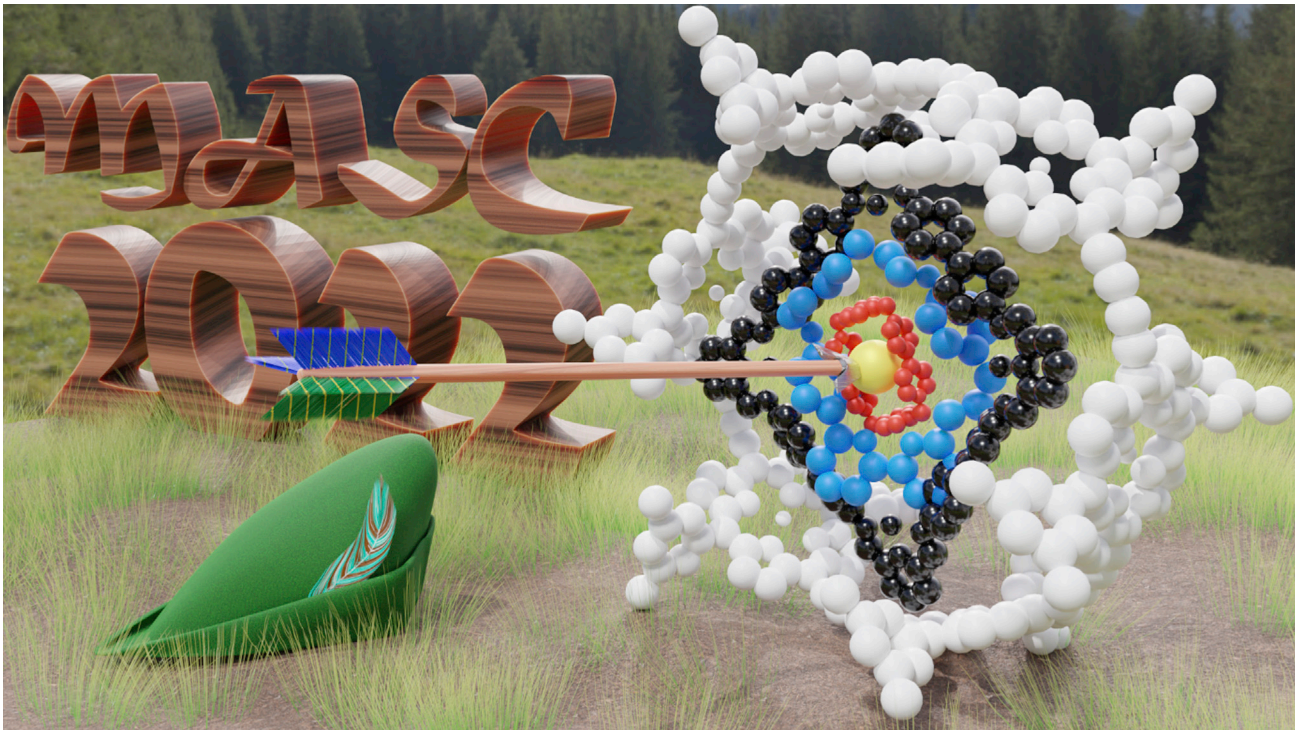
Voices

MASC 2022: What challenges and opportunities do supramolecular chemists face in coming years?

Supramolecular chemistry has gone from strength to strength in recent decades, with its impact felt from catalysis to materials science to chemical biology. This Voices article, published to coincide with the 2022 Macrocyclic and Supramolecular Chemistry Group meeting at the University of Nottingham, UK, asks speakers from the meeting: what are the major challenges and opportunities facing the field in coming years?



Ben S. Pilgrim
School of Chemistry, University of Nottingham, UK

Introduction from the chair

It is a delight to chair the 2022 edition of the Royal Society of Chemistry (RSC)'s Macrocyclic and Supramolecular Chemistry (MASC) Group meeting in the University of Nottingham, the first such meeting in person since 2019. The MASC group, which sees its 40th anniversary this year, had its roots in macrocyclic chemistry. Our meeting logo pays homage to some of the pioneering macrocyclic chemistry undertaken in the UK, in addition to the legendary local archer and outlaw Robin Hood.

The term "supramolecular" came later, but today it has one of the widest remits in chemistry. It's impossible to summarize the breadth of modern supramolecular chemistry on display at this conference: supramolecular materials both hard and soft, both discrete and extended; fundamentals of non-covalent interactions; mechanical bonds; self-assembly; host-guest chemistry; molecular machines; and the interface of supramolecular chemistry with biology. No one can be an expert in all these disciplines, hence the value of broad meetings such as this.

Interactions are key to chemistry, and, in many cases, those conducted at longer distances are weaker. The same is true of interactions between members of our

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community. For the field to progress, we need to collaborate and exchange ideas to make the most of our varied skillsets. Virtual events over the past few years have been crucial to keep the field connected and have been transformative for diversity, equity, and inclusion (DEI) for those unable to attend in-person meetings. These online meetings are here to stay, and, for these reasons, we are also showing talks from MASC 2022 online. Nevertheless, it is hard to virtually recreate the spontaneity of in-person interactions. I hope the discussions and exchange of ideas at this meeting will spark new connections and collaborations to help supramolecular chemistry address the challenges of the 21st century.

Anna Slater
Materials Innovation Factory and Department of Chemistry, University of Liverpool, UK

Supramolecular chemistry is set to benefit from technology

Ensuring reproducibility and scalability of supramolecular syntheses is a significant challenge. The non-covalent and/or reversible processes ubiquitous in the field can be difficult to control, mainly due to their sensitivity to environmental conditions. Selectivity and yield can be poor; batch-to-batch variability can be high and difficult to understand: the number of variables that might make a difference means the parameter space of even simple systems can be vast. High-dilution conditions, templating strategies, and complex synthetic routes can help overcome these challenges but in turn limit the scalability of the process—limiting widespread use of new materials.

Standard tools for the chemist—i.e., round-bottomed flasks—do not offer fine control over environmental parameters or rapid exploration of chemical parameter space. There is a need for tools that enable: (1) greater control over reaction conditions, (2) faster and more extensive exploration of chemical space, and (3) scalable, efficient, and sustainable synthesis. Such tools include high-throughput screening, flow chemistry, and automated techniques. Together with Rebecca Greenaway at Imperial College London, we have written on this in more depth recently (https://doi.org/10.3389/fchem.2021.774987).

Key to the success of these newer techniques is communication between disciplines, training opportunities for researchers, and case studies of how these strategies can be successfully implemented in a supramolecular setting. Equally important are computational strategies to handle large datasets and to model and predict what might be most interesting to screen. Working alongside established supramolecular methods, these tools might make the life of the supramolecular chemist easier—and lead to new insights alongside scalable, sustainable supramolecular chemistry.

Beatrice Collins
School of Chemistry, University of Bristol, UK

New synthetic methods will power the next generation of molecular machines

Many of nature's magnificent motor proteins, such as kinesin and dynein, are powered by the same chemical transformation: the hydrolysis of adenosine triphosphate. The remarkable advances made in the development of autonomously operating chemically fueled molecular motors in recent years have also relied exclusively on a common chemical transformation: the formation and cleavage of acyl linkages. As we look to the design of the next generation of molecular machines, we must harness our power as synthetic chemists and exploit the diverse range of chemical reactivity at our disposal.

The development of new synthetic methodologies continues apace, with highly elegant and sophisticated methods enabling novel bond constructions under mild and often catalytic conditions and with exquisite levels of chemo-, regio-, and stereoselectivity. From transition metal and photoredox catalysis to biocatalysis and electrochemistry, these new methodologies have allowed chemists to explore new

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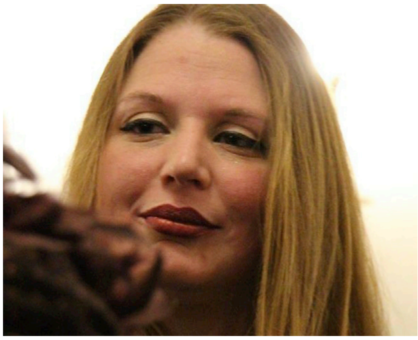
regions of three-dimensional chemical space and tackle energetically challenging transformations in increasingly sustainable ways. The exploitation of these novel methods within the field of molecular machines, however, has been limited. This is despite the fact that many new synthetic methodologies exhibit elements that are essential in the development of autonomously operating molecular motors: multiple processes occurring concurrently, the co-existence of reactive intermediates, and the (catalyst-mediated) modulation of reagent reactivities.

Expanding the toolbox of reactivities that we harness will not only allow identification of new designs for the development of the next generation of nanoscale machines but also open the field to a new generation of molecular machinists.



Jennifer Hiscock
School of chemistry and Forensic science,
University of Kent, UK

Open conversations change supramolecular chemistry for the better

Scientifically, I believe for this field to grow and produce the impact that it deserves, supramolecular innovations need to continue to translate into the commercial space. There are of course current examples of this, but selfishly, I would like to see more. However, I also think that this field should take the time to reflect on the amazing steps forward made over the last three years at both the national and international level to support DEI within science. Of course, more can always be done, but we should celebrate what has been achieved. Since mid-2019, MASC events have included opportunities within their main program to openly discuss issues associated with DEI, providing space for invited presentations and panel discussions, inclusive of the entire community. The success of these events has led to similar events being hosted at other supramolecular chemistry conferences around the world, in particular at the 2022 International Symposium on Macrocyclic and Supramolecular Chemistry (ISMSC), held in Oregon.

Here, I would like to extend my personal thanks to every person who has attended, supported, or enabled events and/or the community activities initiated by the Women in Supramolecular Chemistry (WISC) network. You have all enabled what I believe to be ground-breaking change within our field, and I cannot wait to see how this wave could propagate both within and beyond supramolecular chemistry.

Jennifer Leigh
Centre for the Study of Higher Education,
University of Kent, UK

Increasing inclusivity and equity in research cultures

One of the biggest challenges in science is addressing the widely acknowledged lack of DEI. This is a global challenge including the overrepresentation of European and North American science and scientists. Within chemistry, professional bodies such as the Royal Society of Chemistry and the American Chemical Society showed that compared with what is seen in the general population, there is an underrepresentation of chemists who are women, disabled, Black, Indigenous, and people of color. This gap increases with seniority.

Marginalization can be thought of as being *intersectional* (a term coined by Kimberlé Crenshaw to describe the compounding barriers faced by Black women due to misogyny and racism). Practically, this means that the disadvantages encountered due to different aspects of an individual's identity, such as gender, sexuality, race, religion, or class, will compound and multiply. The competitive climate of scientific research funding reinforces an ideology where overwork and hyperproductivity are the norm. Coupled with increases in precarious contracts, squeezes on budgets, and a lack of progression opportunities, it becomes harder to change the dominant research culture and make it more accessible and inclusive.

Supramolecular chemistry has welcomed the International Women in Supramolecular Chemistry (WISC) network's approach to DEI, responding to them "calling in" the community to support their own and incorporating creative approaches to highlight and humanize the lived experiences of parents, carers, and marginalized researchers. The framework that the community is constructing to raise awareness and effect change could act as a model for other fields within physical sciences to address inclusivity and equity in research cultures.

Jonathan Sessler
Department of Chemistry, The University of Texas at Austin, USA

Advancing separations at the nexus between supramolecular and materials chemistry

Supramolecular chemistry is no longer a single field. Rather, it is a concept that animates modern science from mechanistic biology to molecular machines and organocatalysis. It is thus likely impossible to predict where the future lies. However, one important growth area is in separations. Key contributions have already been made in radioactive waste remediation and metal beneficiation. Promising developments are being made in gas and small molecule separations and in ion pair sequestration. More advances are sure to come as supramolecular chemists tackle current challenges in greenhouse gas capture, water purification, and pollution control. It is our view that progress in separations can be accelerated by exploring the nexus between supramolecular and materials chemistry. In particular, we suggest that polymers bearing suitably selected receptors, either appended to the backbone or incorporated directly into the polymeric chain, will allow improvements in separations. This is because receptor-functionalized materials are expected to benefit from multivalency, where the synergistic participation of multiple recognition motifs leads to enhanced binding. Receptor-containing polymers are also expected to be readily separated from source phases containing the species of interest. This will facilitate use and avoid, for instance, the formation of emulsions under conditions of liquid-liquid extraction-based separations. Recent work from our laboratory has illustrated the viability of this approach. However, we believe that the nexus between supramolecular and materials chemistry remains largely unexplored in the context of separations. This means that the best is yet to come.

Letizia Liirò Peluso
School of Chemistry, University of Nottingham, UK

Supramolecular composition and devices for energy conversion

Chirality of molecules at the surface of supramolecular materials offers a unique way to tune the performance and efficiency of optoelectronic devices for energy conversion. In the flourishing field of organic-based bulk heterojunction photovoltaics based on low-band-gap polymers and non-fullerene small molecules, laboratory-scale layered solar cells are exceeding efficiencies of 18%. The next step change in device performance, and likely in commercialization, might rely on the discovery of synergic effects in the infinite combinations of organic materials (composing the photo-active layer, PAL), thin film layers, and interfaces.

Aspects of device performance, such as durability, can be enhanced through careful manufacture, but the key to functionality lies in the control and maintenance of the supramolecular composition of the PAL. This can allow the fundamental processes of light absorption, exciton dissociation, and charge transport/recombination to be effectively controlled. One way in which the PAL can be modified to optimize device performance is through the controlled supramolecular assembly of organic materials that absorb and emit circularly polarized light in the solid state. Such systems have the potential to deliver cell efficiencies that far exceed the state of the art. Although significant challenges remain in optoelectronics, supramolecular chemistry offers us a route toward a more sustainable energy future.

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Supramolecular chemistry will unlock new CPL-active materials

There has been a significant growth in recent years of research concerning chiral organic and hybrid thin film materials. Such interest stems, in part, to the ability to use such materials for the selective absorption or emission of a helically chiral polarization state of light: circularly polarized light (CPL). Downstream applications resulting from CPL-active films span many areas, from high-performance displays to encryption and quantum information processing. One key challenge for this field, however, is the fact that current and emerging chiral chromophoric molecules only have very weak chiroptical activity; that is to say that selectivity in the absorption or emission of one CPL handedness over the other is very low. The ability to mediate a *highly selective* chiroptical response is essential to realize the translational opportunities highlighted above. One significant opportunity to enhance the chiroptical activity of a chiral chromophore is through supramolecular chemistry. For example, we have shown that conjugated polymer thin films, when assembled into helical bundles, can result in very large intrinsic chiroptical activity through excitonic coupling between adjacent polymer chains in the supramolecular assembly. Furthermore, we have recently shown that templating layers, together with vacuum deposition, can be used to control the directionality of supramolecular columns of helical small molecules. This directionality can, in turn, be used to control the chiroptical response. While other approaches continue to be discovered in this exciting area, one fact is apparent: considerations beyond the molecule will be key to unlocking materials and applications involving CPL.

Tomislav Friščić
School of Chemistry, University of Birmingham, UK

Mechanochemistry offers both synthetic challenges and opportunities

Over the past 20 years, mechanochemical reactions, driven or initiated by mechanical agitation in the form of milling, grinding, or extrusion, have evolved from a laboratory curiosity into a cornerstone of cleaner, safer, and more effective synthesis. Benefits of mechanochemistry have been demonstrated in many areas of chemical and materials synthesis, from zeolites and other types of framework materials to hybrid perovskites, catalysis, organometallics, pharmaceuticals, and more. Such developments have been accompanied by the creation of international collaborations and centers, as exemplified by the National Science Foundation Centre for Mechanical Control of Chemistry, the EU COST Action Project for Mechanochemistry for Sustainable Industry, and, very recently, the Impactive Consortium.

Such global interest in mechanochemistry now highlights important challenges that must be overcome to fulfill the potential of the field in sustainable, greener manufacturing. These include developing technologies that enable scaling up of mechanochemical processes with minimal re-optimisation—advances are already being made in that area, and our experiences highlight that new media-free techniques, such as resonant acoustic mixing and SpeedMixing, have a lot going for them. The second major challenge of mechanochemistry is fundamental understanding of the underlying processes, specifically focusing on how to model them and to, ultimately, predict them. This area is still very much in its infancy, but strides are being made in applications of periodic density-functional theory and molecular dynamics toward that goal. Overcoming these two challenges will enable chemists to deliberately design new reactions, and immediately scale them up for manufacturing: a dream yet to be accomplished.

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Functional systems from self-assembled supramolecular toolkits

The development of highly complex and beautiful, yet functional and application-based, structures is a particular highlight of supramolecular and macrocyclic chemistry. In recent years, an increased focus on supramolecular utility, such as encapsulation, catalysis, and mechanical work, has expanded the scope of this interdisciplinary research area. However, a major enduring challenge is the significant synthetic effort required to realize many such systems; to combat this, minimalist assemblies should be targeted while we continue to develop new synthetic strategies and supramolecular toolkits. The extraordinary power of self-assembly will undoubtedly continue to be utilized to this effect. Additionally, recent progress toward increasingly intricate supramolecular machines highlights our still-limited understanding of complex and non-equilibrium systems, and this necessitates greater collaboration between theoretical, experimental, and computational resources. The future direction of the field of supramolecular chemistry could see, for example, nanoscale motifs matching their macroscale counterparts in specificity and efficiency, such as precise encapsulation of any guest on demand within molecular cages, or nanoscale knots optimized for exact functions. By continuing to look to nature for inspiration, particularly in the areas of compartmentalization, transportation, and out-of-equilibrium systems, the field of supramolecular chemistry has the potential to make a true difference within the most pressing scientific challenges.

DECLARATION OF INTERESTS

The authors declare no competing interests.