

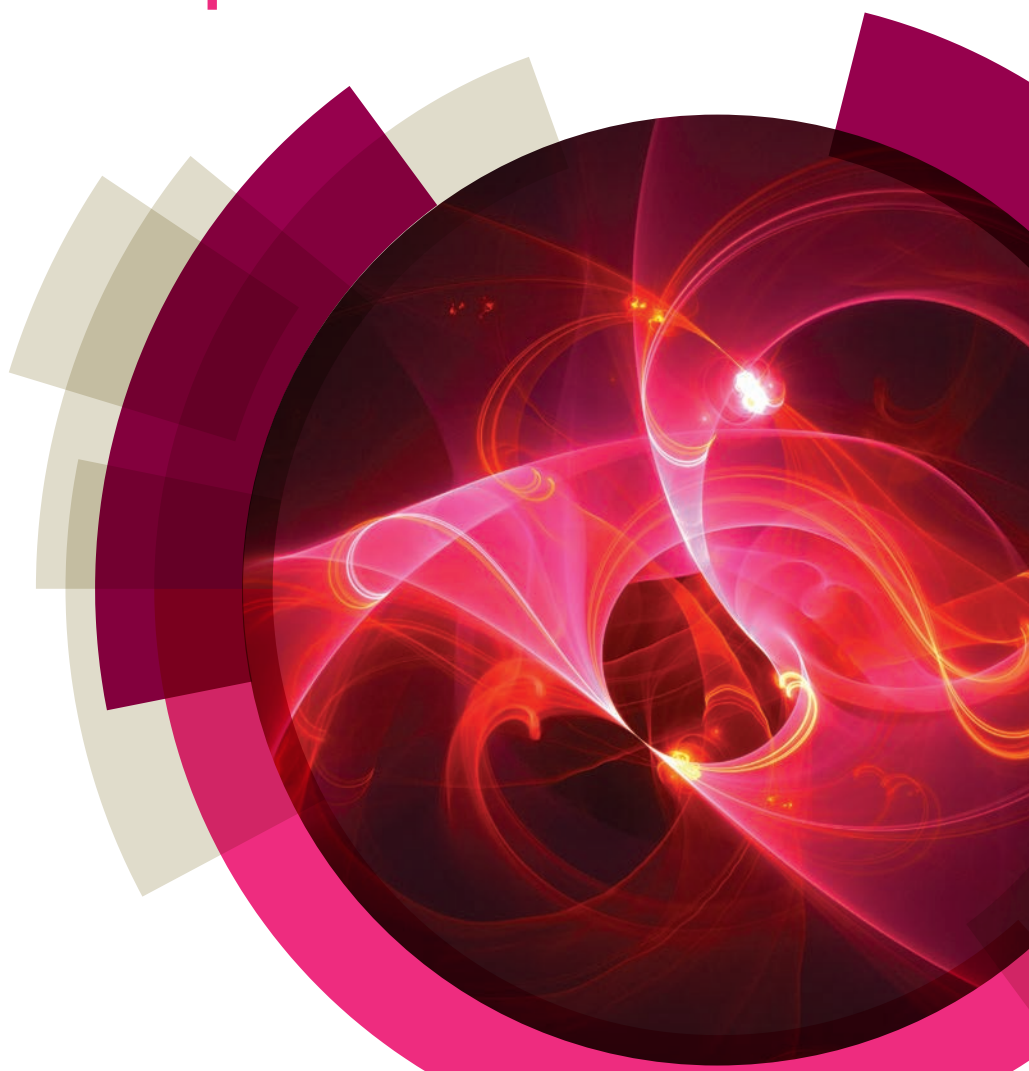


1 October 2018, London

# 9th Joint CSJ RSC Symposium: Designing Molecular Function at the Nano-Scale: Catalysis, Materials and Supramolecular Chemistry

## Book of Abstracts

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## Welcome address from the Royal Society of Chemistry

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Dear Colleagues

It is my pleasure as Past-President of the Royal Society of Chemistry to welcome you to the 9th Joint CSJ RSC Symposium on Designing Molecular Function at the Nano-Scale: Catalysis, Materials and Supramolecular Chemistry. A particularly warm welcome to Professor Maki Kawai, President of the Chemical Society of Japan, and our Japanese speakers, all of whom have made the long journey to the UK to be with us today.

The Royal Society of Chemistry has worked closely with the Chemical Society of Japan for a number of years to support scientific collaboration and exchange between our two countries. In 2010 we formalised our relationship by signing an international cooperation agreement, which we renewed in 2015. This symposium is the latest in a series of successful joint symposia that we have organised as part of this relationship. Five years ago, in 2014, I had the pleasure of addressing the 5th Joint CSJ RSC Symposium on Supramolecular Chemistry, an area not dissimilar to that of today's symposium. I am especially looking forward to hearing from our invited speakers on the latest advances in the fields of catalysis, materials and supramolecular chemistry, and how these areas can be applied to design molecular function at the nano-scale.

I would like to thank the Chemical Society of Japan, particularly its President Professor Maki Kawai, Executive Director Professor Mitsuo Sawamoto and International Relations Officer Ms Emiko Sakurada for their contribution to today's event. My thanks also go to Professor Jonathan Clayden and Professor Seiji Shirakawa for assembling such an impressive programme representing some of the latest Japanese and UK research in this area of chemistry – thank you to each of the speakers and all the participants for their contributions to this symposium. Finally I would like to thank the UK research groups who have kindly arranged for some of our Japanese guests to visit their institutions during their time in the UK. Chemistry of course is, and must always remain, collaborative and international, and events such as this give participants the opportunity to exchange ideas, forge new friendships and embark on joint collaborations. I hope that today offers yet more opportunities for researchers from the UK and Japan to collaborate on this important topic.

Once again a very warm welcome to what promises to be an exciting scientific event. I wish you all an informative, productive and enjoyable day.



Professor Lesley Yellowlees CBE, FRSE, HonFRSC  
Past-President  
*Royal Society of Chemistry*

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## Welcome address from the Chemical Society of Japan

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Dear Colleagues

Welcome to the 9th Joint CSJ RSC Symposium on Designing Molecular Function at the Nano-Scale: Catalysis, Materials and Supramolecular Chemistry. It is my pleasure as President of the Chemical Society of Japan to be with you today.

The Chemical Society of Japan (CSJ) and Royal Society of Chemistry (RSC) have collaborated on many successful joint activities. Our interdisciplinary symposia offer a unique platform by bringing together scientists from different disciplines in Japan and the UK to share ideas and experiences.

Supramolecular chemistry has been and continues to be an area of particular focus for us in creating new and interesting functional materials. In 2014 our two societies organized a joint symposium on supramolecular chemistry. In today's symposium we will hear how the fields of catalysis, materials and supramolecular chemistry can be applied to the areas of molecular space and design and new materials function.

Functional space is an important material component for molecular recognition and catalysis. A series of zeolites of differing pore sizes ranging from the sub-nanometer to micron-meter scale can be used for a wide range of applications. Using a supramolecular chemistry approach to synthesize homogeneous and precisely designed materials has the potential to enable the known pore function of materials to functionalize each site of the pore with a view to producing new types of control materials.

I would like to thank Professor Seiji Shirakawa, Professor Yoshinori Takashima and Professor Jonathan Clayden for suggesting and refining the topic of the symposium, and for inviting so many excellent speakers to present their work to us today. I believe this opportunity to sit together at the same table will provide a meaningful chance for sustainable collaboration between our two countries.



Professor Maki Kawai  
President  
*Chemical Society of Japan*

## Programme

Time	Event	Chair
09:30	Registration and coffee	
10:15	<b>Welcome remarks</b> Professor Lesley Yellowlees <i>Past-President, Royal Society of Chemistry</i> Professor Maki Kawai <i>President, Chemical Society of Japan</i>	Dr Robert Parker <i>CEO, Royal Society of Chemistry</i>
10:30	<b>Design of organo-sulfur catalysts</b> Seiji Shirakawa	Jonathan Clayden
10:55	<b>Asymmetry from the mechanical bond: Synthesis and applications of “mechanically” chiral molecules</b> Steve Goldup	
11:20	Coffee break	
11:35	<b>Development of chirality-switchable functional materials based on the solvent-dependent inversion of the main-chain helical chirality</b> Yuuya Nagata	Seiji Shirakawa
12:00	<b>Synthetic mimicry of biological communication devices</b> Jonathan Clayden	
12:25	<b>Exploring new concept for the use of sulfur in the molecular design of functional Pi-electron materials</b> Aiko Fukazawa	
12:50	Lunch and poster session	
14:15	<b>Pillar-shaped macrocyclic compounds “pillar[n]arenes”: From simple molecular receptors to bulk supramolecular assemblies</b> Tomoki Ogoshi	Steve Goldup
14:40	<b>Functional structures via subcomponent self-assembly</b> Jonathan Nitschke	
15:05	<b>Catalytic function dictated by the B<sub>3</sub>NO<sub>2</sub> ring system</b> Naoya Kumagai	
15:30	Coffee break	
15:45	<b>C-H functionalisations: Palladium, gold, light, dark?</b> Ai-Lan Lee	Aiko Fukazawa
16:10	<b>Supramolecular polymeric materials functionalized by host-guest interactions and its stimuli-responsive properties</b> Yoshinori Takashima	
16:35	<b>Template-directed synthesis and electronic delocalization in molecular nanocages and nanorings</b> Harry Anderson	
17:00	<b>Presentation of poster prizes</b>	Ai-Lan Lee
17:10	<b>Closing remarks</b> Mr Paul Lewis <i>Deputy CEO, Royal Society of Chemistry</i>	
17:30	Networking reception	



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## Biographical notes of invited speakers

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**Harry Anderson**

*University of Oxford, UK*

Email: [harry.anderson@chem.ox.ac.uk](mailto:harry.anderson@chem.ox.ac.uk)

Harry Anderson obtained his BA in chemistry from the University of Oxford under John M. Brown and his PhD in chemistry from the University of Cambridge under Jeremy K. M. Sanders. He held postdoctoral research fellowships at Magdalene College Cambridge (1990-1993) followed by ETH- Zürich (1993-1994), before moving to Oxford in 1994 to become a lecturer in organic chemistry. He was a Tutorial Fellow at Keble College from 1994-2013 and has been a Professorial Fellow since October 2013. He has published more than 280 research articles in peer-reviewed journals, and is interested in molecules with extended  $\pi$ -systems and supramolecular self-assembly. He has received the 2001 Corday-Morgan Award (Royal Society of Chemistry), 2003 Bob Hay Lecturer (Royal Society of Chemistry, Macrocyclic Chemistry), 2003 Award for Materials Chemistry (Royal Society of Chemistry), 2006 Award for Supramolecular Chemistry (Royal Society of Chemistry), 2012 Tilden Prize (Royal Society of Chemistry), 2013 ERC Advanced Investigator Award, and the 2017 Izatt-Christensen Award for Macrocyclic and Supramolecular Chemistry. He has also held a number of lectureships throughout his career, including the 2013 Alexander Todd – Hans Krebs Lectureship (RSC/GDCh). He is a fellow of the Royal Society (elected 2013) and the Royal Society of Chemistry (elected 2003), an Honorary Member of the Israel Chemical Society (2014) and a member of the American Chemical Society.



**Jonathan Clayden**

*University of Bristol, UK*

Email: [j.clayden@bristol.ac.uk](mailto:j.clayden@bristol.ac.uk)

Jonathan Clayden was born in Uganda in 1968, grew up in the county of Essex, and was an undergraduate at Churchill College, Cambridge. In 1992 he completed a PhD at the University of Cambridge with Dr Stuart Warren. After postdoctoral work with Professor Marc Julia at the École Normale Supérieure in Paris, he was appointed as lecturer at the University of Manchester in 1994. In 2001 he was promoted to professor, and in 2015 he moved to the University of Bristol. He has published 270 papers, and his research interests encompass areas of synthesis and stereochemistry where conformation has a role to play: dynamic foldamers, atropisomerism, organolithium chemistry, conformationally-induced reactivity and long-range stereochemical effects. He pioneered the field of dynamic foldamer chemistry, using molecular conformational features to devise synthetic mimics of biological communication devices, including an artificial membrane-bound receptor and a mimic of the vision protein rhodopsin, and he has established the feasibility of stereochemical control over nanometre distances. His work on conformationally induced reactivity has led to new dearomatisation, arylation, and ring expansion chemistry applicable to the synthesis of challenging targets of actual and potential biological activity. He is a co-author of the widely used textbook "Organic Chemistry" published by OUP, and his book "Organolithiums: Selectivity for Synthesis" was published by Pergamon in 2002. He has received the Royal Society of Chemistry's Meldola (1997) and Corday Morgan (2003) medals, Stereochemistry Prize (2005), Hickinbottom Fellowship (2006), Merck Prize (2011) and Tilden Award (2018), and the Novartis Young European Investigator Award (2004). He has held an ERC Advanced Grant and has been awarded senior research fellowships from the Leverhulme Trust and the Royal Society.

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**Aiko Fukazawa**

*Nagoya University, Japan*

Email: aiko@chem.nagoya-u.ac.jp

Aiko Fukazawa studied chemistry at Kyoto University where she obtained her B. Eng. degree and M. Eng. degree in 2002 and 2004, respectively, under the supervision of Professor Kohei Tamao. On the way to pursuing her doctorate at the same university, she moved to Professor Shigehiro Yamaguchi's research group in Graduate School of Science at Nagoya University as an assistant professor in 2006, received her Dr. Sci. from Nagoya University in 2008, and promoted to an associate professor in August 2013. She also spent two months to work with Professor Warren E. Piers at University of Calgary as a visiting scholar in 2011. Since April 2013, she has been concurrently serving as a collaborating investigator in the Institute of Transformative Bio-Molecules in Nagoya University. Based on her achievements in the field of main-group chemistry, she received several awards including Inoue Research Aid for Young Scientists (2009), Asian Core Program Lectureship Award to Taiwan and Singapore (2010), The Chemical Society of Japan Award for Distinguished Young Chemists (2014), and Nozoe Young Scientist Award (2017). Her research interests include the development of novel functional organic materials on the basis of physical organic chemistry and main group chemistry.



**Steve Goldup**

*University of Southampton, UK*

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I studied at the University of Oxford (MChem, Prof. Sir Jack Baldwin) and Imperial College (PhD, Prof. Tony Barrett) where my research focused on natural product synthesis, before moving to Edinburgh (PDRA, Prof. David Leigh) to apply my synthetic skills to interlocked molecules and molecular machines. In 2008 I took up my first independent research position at Queen Mary, University of London, first as a Leverhulme Trust Early Career Fellow and then as a Royal Society Research Fellow and Senior Lecturer. In 2014 I moved to the University of Southampton where I am now Professor of Chemistry. I work with an outstanding group of young scientists demonstrating new applications of interlocked molecules in a range of areas including catalysis, materials, sensing and chemical biology. We are particularly interested in the applications of new forms of stereochemistry associated with the mechanical bond.

**Naoya Kumagai***Institute of Microbial Chemistry, Japan*

Email: nkumagai@bikaken.or.jp

Naoya Kumagai was born in 1978 and raised in Ibaraki (Japan). He obtained his bachelor's (2000), Master's (2002), PhD degrees (2005) in pharmaceutical sciences at The University of Tokyo (Japan), under the supervision of Professor Masakatsu Shibasaki. He received JSPS research fellowships for young scientists (2002–5). He pursued postdoctoral studies in the laboratory of Professor Stuart L. Schreiber at Harvard University (USA) in 2005–6. He moved back to Professor Shibasaki's group at The University of Tokyo as an assistant professor in 2006. He moved to the Institute of Microbial Chemistry (Tokyo, Japan) together with Prof. Shibasaki in 2010 and is currently a Chief Researcher. He is a recipient of the Pharmaceutical Society of Japan Award for Young Scientists (2010), Thieme Chemistry Journals Award (2013), Young Scientists' Prize, The commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology (2013), and Mitsui Chemicals Catalysis Science Award of Encouragement (2014), and Merck-Banyu Lectureship Award (2017). His research interests include the development of new methodologies in catalysis, design & synthesis of exotic molecular architectures.

**Ai-Lan Lee***Herriot-Watt University, UK*

Email: A.Lee@hw.ac.uk

Ai-Lan was born in Malaysia and obtained her MSci (Hons) (2000) and PhD (2004) from University of Cambridge, working under the supervision of Prof. Steven V. Ley. She was subsequently awarded a Lindemann Trust Fellowship (2004–2005) to work at Boston College with Prof. Amir Hoveyda on alkene metathesis. In 2006, Ai-Lan was appointed as a fixed-term Lecturer at the University of Edinburgh, carrying out research with Prof. David Leigh on rotaxane synthesis. She started as a Lecturer at Heriot-Watt University in 2007 and is currently Associate Professor and Reader. Her research interests include developing new gold-, palladium- and dual photoredox-catalysed reactions.

**Yuuya Nagata***Kyoto University, Japan*

Email: nagata@sbchem.kyoto-u.ac.jp

Yuuya Nagata is an Assistant Professor at Kyoto University. He studied polymer chemistry at Kyoto University, obtaining his PhD under the supervision of Prof. Yoshiki Chujo in 2008. Later, he joined Prof. Michinori Suginome's group at Kyoto University. His interest is focused on the science of helical polymers to figure out the nature of chirality. In particular, he is interested in the synthesis and the screw-sense control of poly(quinoxaline-2,3-diyl)s, which exhibit various molecular functions including asymmetric catalysis and generation of circular polarized light. He is also interested in the use of various techniques to investigate helical polymers, including neutron beam scattering, synchrotron X-ray scattering and diffractions, high-pressure circular dichroism measurements, and large-scale theoretical calculations. He has been awarded several prizes, including the Special Lecturer for Young Chemists (the Chemical Society of Japan, 2015), the Young Scientist Presentation Award (the Society of Polymer Science, Japan, Kansai Regional Chapter, 2015), and the CSJ Award for Young Chemists (the Chemical Society of Japan, 2017).





**Jonathan Nitschke**  
*University of Cambridge*  
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Jonathan Nitschke received his bachelor's degree from Williams College (USA) in 1995 and his doctorate from the University of California, Berkeley in 2001 under the supervision of T. Don Tilley. He then undertook postdoctoral studies with Jean-Marie Lehn in Strasbourg under the auspices of a US NSF fellowship, and in 2003 he started his independent research career as a Maître-assistant (fixed-term independent PI) in the Organic Chemistry Department of the University of Geneva. In 2007 he was appointed University Lecturer at Cambridge, where he now holds a Professorship. His research program investigates the self-assembly of complex, functional structures from simple molecular precursors and metal ions.



**Tomoki Ogoshi**  
*Kanazawa University, Japan*  
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Tomoki Ogoshi received his B.S. (2000), M.S. (2002), and Ph.D. degrees (2005) from Kyoto University under the supervision of Prof. Yoshiki Chujo. He was a JSPS postdoctoral research fellow (2005–2006) in the Graduate School of Science at Osaka University in the group of Prof. Akira Harada. In 2006, he moved to the Graduate School of Natural Science and Technology at Kanazawa University as an assistant professor (2006–2010). He was an associate professor (2010–2015) and was promoted to a professor at the same university at 2015. He works also as JST-PRESTO Researcher: PRESTO program "Hyper-nano-space design toward innovative functionality" from Oct. 2013 under the research supervisor of Prof. Kazuyuki Kuroda (Waseda University). He was a visiting professor at University of Amsterdam (co-worker: Albert M. Brouwer, May 2017–Jan. 2018). He has received HGCS Japan Award Excellence 2010 (2011), The Chemical Society of Japan Award for Young Chemists (2012), The Cram Lehn Pedersen Prize in Supramolecular Chemistry; Royal Society of Chemistry (2013), The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology (2014), Nozoe Memorial Award for Young Organic Chemists (2016), Banyu Chemist Award 2016 (2016) and Lectureship Award MBLA 2016 (2017). His research interests include organic synthesis, and supramolecular and hybrid materials.



**Seiji Shirakawa**

*Nagasaki University, Japan*

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Seiji Shirakawa was born in 1974 in Ehime, Japan. He graduated from Nihon University (1997) and received his Ph.D. (2004) from Kyoto University under the supervision of Professor Keiji Maruoka. He worked with Professor James L. Leighton at Columbia University (2004–2005) and Professor Shū Kobayashi at University of Tokyo (2005–2007) as a postdoctoral fellow. He was appointed as an assistant professor at Nihon University in 2007, and moved to Kyoto University as an associate professor (2009). He is currently an associate professor in Nagasaki University since 2014. He has received The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, The Young Scientists' Prize (2013), Incentive Award in Synthetic Organic Chemistry, Japan (2014), and Nagase Foundation Award (2015). His research interests include supramolecular catalysis, onium salt catalysis, and organo-sulfur catalysis.



**Yoshinori Takashima**

*Osaka University, Japan*

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Yoshinori Takashima was born in 1974 in Osaka, Japan. He received his Ph.D. degree in 2002 from Osaka University, under the guidance of Prof. Akira Harada (Osaka Univ.), focusing on the polymerization catalyst using group 4 transition metal catalyst. He was selected as a Research Fellow of the Japan Society for the Promotion of Science (JSPS) in 1999–2002. During the winter of 2003, as a visiting fellow, he worked at Prof. Jeffrey M. Stryker's lab, Department of Chemistry, the Univ. of Alberta. In 2003, he obtained his PhD in Polymer Science from Osaka Univ. Prior to joining the Graduate School of Science at Osaka Univ. in 2004 as an assistant prof. for Prof. Akira Harada, he served as a postdoctoral research fellow from JSPS in the Division of Applied Chemistry, Osaka Univ. for Professor Toshikazu Hirao. In 2011, he worked at Prof. Philip A. Gale's lab, Department of Chemistry, the Univ. of Southampton as a visiting researcher. In 2016, he joined the Graduate School of Science at Osaka Univ. as a lecturer. In 2018, he visited to Prof. Nicolas Guiseppone of the Univ. of Strasbourg as a visiting professor. At the same year, he joined Institute for Advanced Co-Creation Studies and the Graduate School of Science at Osaka Univ. as a professor. His research interests include supramolecular materials, catalysts, molecular motors and devices.

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# Template-directed synthesis and electronic delocalization in molecular nanocages and nanorings

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Large monodisperse  $\pi$ -conjugated nanostructures based on metalloporphyrins, with sizes similar to those of proteins, are becoming increasingly accessible due to advances in template-directed synthesis. The properties of these systems are just starting to be understood. They are unique model systems for testing electronic delocalization in molecular nanostructures.

This presentation will focus on the synthesis, aromaticity and electronic delocalization in large  $\pi$ -conjugated nanorings, nanotubes and nanoballs constructed from porphyrin units.<sup>2</sup> The spectroscopy of the simple porphyrin nanorings continues to generate surprises,<sup>3</sup> while advances in template-directed synthesis are rapidly providing access to new architectures, such as the 14-porphyrin nanoball shown below (Figure 1), which features two orthogonal intersecting  $\pi$ -conjugated circuits.<sup>4</sup> Results will also be presented on single-molecule charge-transport through these systems.

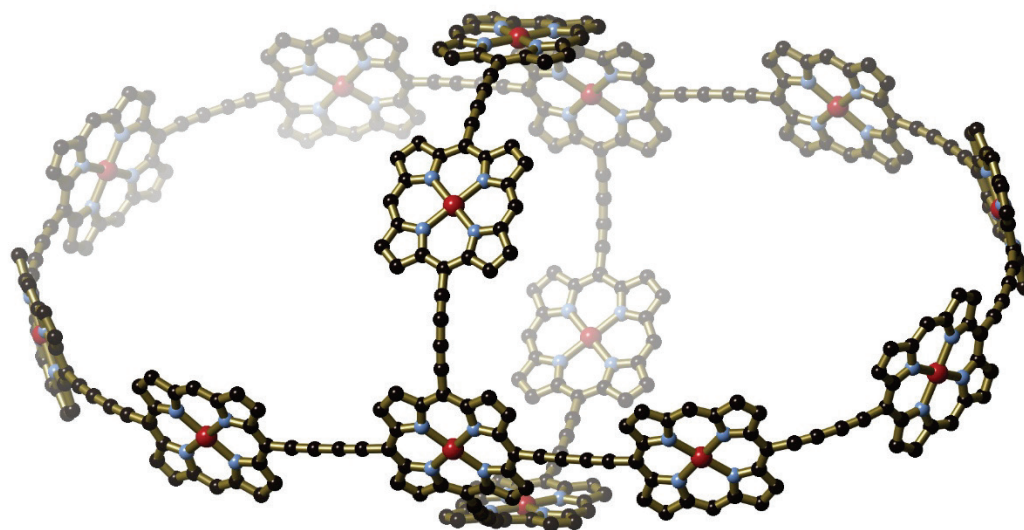


Figure 1. Calculated structure of a  $\pi$ -conjugated nanoball consisting of 14 zinc porphyrin centers. (Hydrogen atoms and solubilizing side groups not shown.)<sup>4</sup>

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## Synthetic mimicry of biological communication devices

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Jonathan Clayden

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Biology communicates information through cell membranes by means of conformationally switchable proteins, of which the most important are the G-protein coupled receptors (GPCRs). This lecture will explore the design and synthesis of artificial mimics of GPCRs, with the ultimate aim of controlling function in the interior of an artificial vesicle. Prospects for future developments of molecular devices capable of encoding information in conformation and translating that information into chemical function will be assessed.

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# Exploring new concept for the use of sulfur in the molecular design of functional $\pi$ -electron materials

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Aiko Fukazawa

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Incorporation of main-group elements into  $\pi$ -conjugated frameworks is one of the promising approaches for the modulation of electronic structures and thus their optical and/or electronic properties. However, this approach often poses a challenge of compromise between unusual electronic structure and chemical stability of the resulting  $\pi$ -systems. In this regard, sulfur-containing  $\pi$ -conjugated systems are attractive class of materials owing to their high stability and attractive electronic properties. Nevertheless, most of the molecular design for thiophene- or TTF-based  $\pi$ -conjugated systems has focused on their electron-donating characters based on the orbital interaction between sulfur lone pair electrons and  $\pi$ -systems. Our idea is to utilize these latent characteristics of sulfur for the molecular design of functional  $\pi$ -electron materials. In this presentation, I will discuss our recent results, including 1) the utilization of the weak aromatic character of thiophenes for the stabilization and activation of highly reactive nonbenzenoid hydrocarbons,<sup>1</sup> and 2) the development of novel solubilizing groups for  $\pi$ -electron systems based on sulfur containing medium rings.<sup>2</sup>

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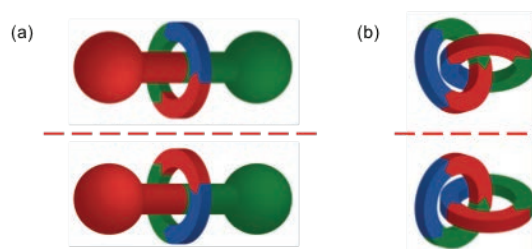
# Asymmetry from the mechanical bond: Synthesis and applications of “mechanically” chiral molecules

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Steve Goldup

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Interlocked molecules can display forms of stereochemistry that do not rely on classical covalent stereogenic units.<sup>1</sup> Our group have pioneered the use of “small” macrocycle<sup>2,3</sup> mediated active template<sup>4</sup> reactions in order to allow the synthesis of challenging interlocked structures,<sup>5,6,7</sup> for applications in sensing<sup>8</sup> and catalysis.<sup>9</sup> Here we describe recent progress in the stereoselective active template synthesis of enantiopure mechanically planar chiral rotaxanes (a)<sup>10</sup> and topologically chiral catenanes (b)<sup>11</sup> for a range of applications.



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## Catalytic function dictated by the B<sub>3</sub>NO<sub>2</sub> ring system

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Naoya Kumagai

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The state-of-the-art chemical toolbox for the amide bond formation deploys a catalytic alternative to allow for dehydrative amidation avoiding the formation of reagent-derived waste, which is never fulfilled by the reagent-driven amidation. While more than two decades have passed since the first manifestation of the catalytic amidation, catalytic protocols have not been widely adopted in practical synthesis due to limited catalytic activity and substrate generality. In particular, embracing  $\alpha$ -amino acids as substrates to catalytically forge amide bonds of peptides, a representative amide-rich chemical entity of significant biological interest, remains challenge to synthetic chemists. The chemical synthesis of peptides is a research area of significant biological and practical impact with high demand, and engineered and expensive coupling reagents are primarily utilized to couple  $\alpha$ -amino acid units for reliable conversion and stereochemical integrity. Herein we introduce an exotic heterocycle DATB (1,3-dioxo-5-aza-2,4,6-triborinane, B<sub>3</sub>NO<sub>2</sub> ring system), a multiboron catalyst amenable for dehydrative direct amidation. DATB is capable of interconnecting a range of carboxylic acids and amines, including sterically demanding substrates, sulfoximines, and all of the natural  $\alpha$ -amino acids. Recent efforts on mechanistic study will be also presented, illuminating the particular activation mode exerted by the peculiar B<sub>3</sub>NO<sub>2</sub> ring system.

## C-H functionalisations: Palladium, gold, light, dark?

Ai-Lan Lee

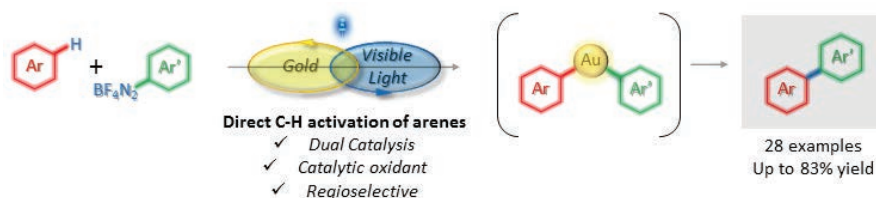
*Institute of Chemical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK*

*A.Lee@hw.ac.uk*

This talk will cover 3 different types of C-H functionalisations developed within the Lee Group: using Pd-catalysis, dual gold and photoredox catalysis, and finally using no catalysis.

**Palladium Catalysis:** A direct Pd-catalyzed C-H functionalisation of benzoquinone (BQ) will be discussed, which can be controlled to give either monosubstituted or disubstituted BQ, including the installation of two different groups in a one-pot procedure.<sup>2</sup> BQ can now be directly functionalized with aryls, heteroaromatics, cycloalkyls and cycloalkenes and, moreover, the process exploits environmentally benign water or acetone as solvents.

**Gold/Photoredox Catalysis:** The merging of photoredox catalysis with gold catalysis is a relatively new yet vibrant field as it enables the access of Au(I)/Au(III) catalytic cycles,<sup>2</sup> and thereby the ability of gold to catalyse cross-couplings without the need for stoichiometric oxidants. Within this context, a mild and fully catalytic aryl-aryl cross coupling *via* gold-catalysed C-H activation has been achieved by merging gold and photoredox catalysis.<sup>3</sup> The procedure is free of stoichiometric oxidants and additives, which were previously required in gold-catalysed C-H activation reactions. One of the key benefits of gold-catalysed C-H activation is regioselectivity, without the need for directing groups. Indeed, we show that exploiting dual gold and photoredox catalysis confers regioselectivity *via* the crucial gold-catalysed C-H activation step, which is not present in the unselective photocatalysis-only counterpart.



**C-H Alkylations, Uncatalysed:** Finally, our recent progress on developing metal, photocatalyst and light-free, late-stage C-H alkylation of heteroarenes and 1,4-quinones using carboxylic acids will be covered.

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# Development of chirality-switchable functional materials based on the solvent-dependent inversion of the main-chain helical chirality

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Increasing attention has focused on the screw-sense control of the polymer backbone for the development of new chiral functional materials, including asymmetric catalysts and chiroptical materials. Recently, we found that poly(quinoxaline-2,3-diyl)s bearing chiral side chain adopts purely single-handed helical conformations, whose helical chirality can be perfectly controlled by the solvents (the solvent-dependent helix inversion, Figure 1a).<sup>1–3</sup> In this presentation, we present the development of new chirality-switchable functional materials based on the solvent-dependent helix inversion of poly(quinoxaline-2,3-diyl)s (Figures 1b and 1c)<sup>4–7</sup> along with the elucidation of the mechanism of the helix inversion.<sup>8</sup>

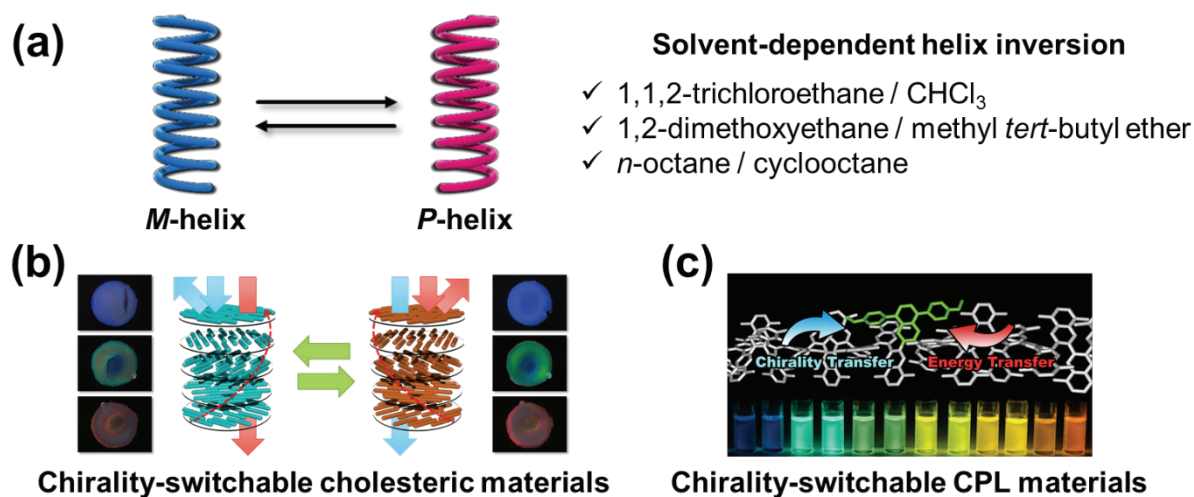


Figure 1. (a) The solvent-dependent helix inversion of poly(quinoxaline-2,3-diyl)s and chirality-switchable (b) cholesteric and (c) circular polarized luminescent (CPL) materials.

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# Functional structures via subcomponent self-assembly

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The materials that we depend on rely upon ever-increasing structural complexity for their function. The use of chemical self-assembly as a synthetic technique can simplify materials preparation by shifting intellectual effort away from designing molecules, and towards the design of *chemical systems* that are capable of self-assembling in such a way as to express desired materials properties and functions. Below are shown the subcomponent precursors and structures of three of products that can form functional constituents of these systems (Figure 1).

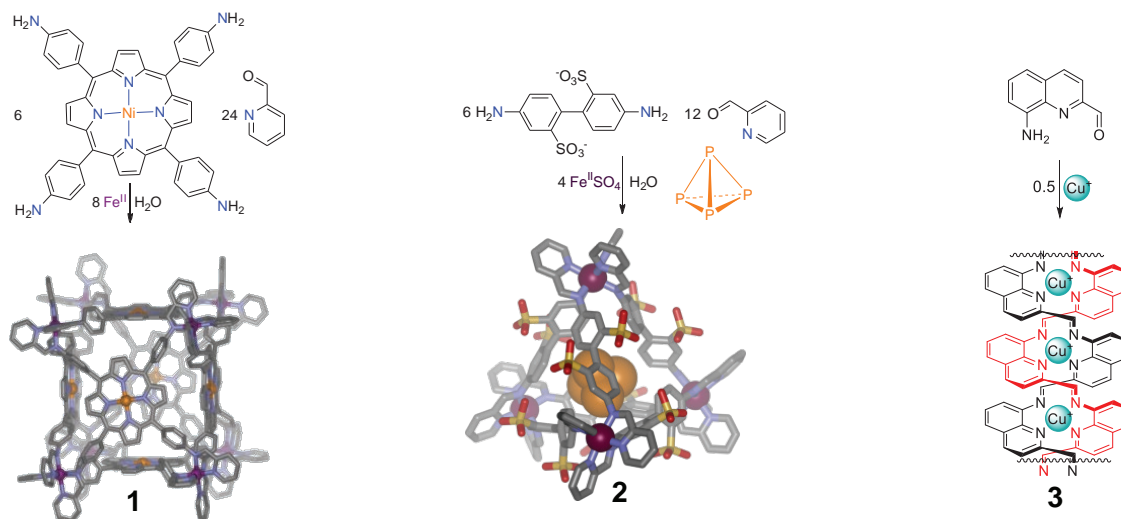


Figure 1.  $\text{Fe}^{\text{II}}$  cubic cage **1**,<sup>1</sup>  $\text{Fe}^{\text{II}}$  tetrahedral cage **2**,<sup>2</sup> and electroluminescent  $\text{Cu}^{\text{I}}$  double-helical polymer **3**<sup>3</sup>

Current challenges involve inducing multiple structures to form in parallel,<sup>4</sup> such that they may act in concert to achieve a catalytic goal,<sup>5</sup> our techniques allow entry into the emerging field of *systems chemistry*.<sup>6</sup> Functional systems that we have recently developed include a fuel-controlled self-assembly process<sup>7</sup> and a series of cages that can phase-segregate<sup>8</sup> and transit between liquid phases.<sup>9</sup>

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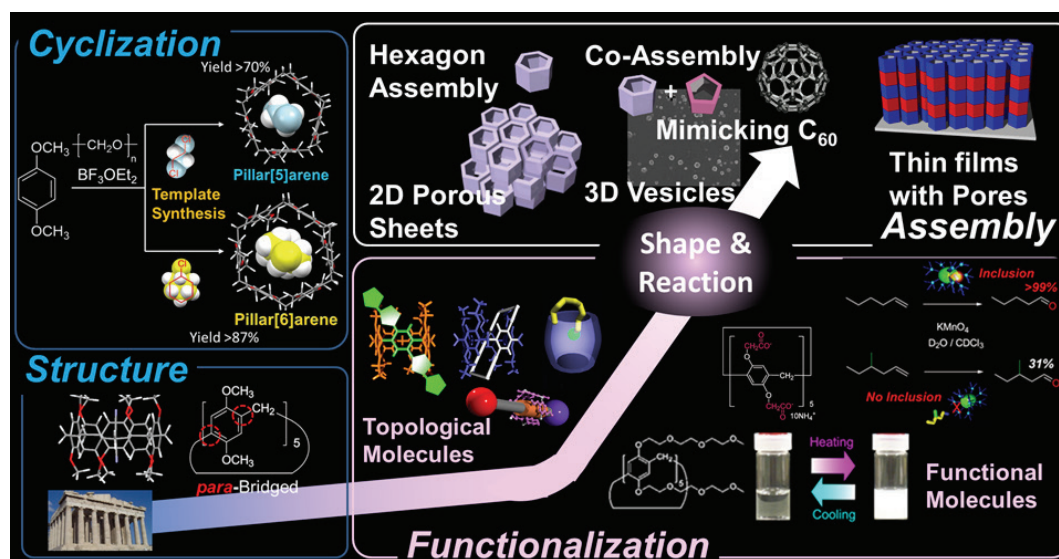
# Pillar-shaped macrocyclic compounds “pillar[n]arenes”: From simple molecular receptors to bulk supramolecular assemblies

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Macrocyclic compounds play a major role in supramolecular chemistry because of their beautiful shape, nano-scale size and molecular recognition ability. Numerous supramolecular architectures have been constructed and studied as new components of materials as well as entities related to biological structural formation and functions using various macrocyclic hosts.

In 2008, we reported a new class of macrocyclic hosts named “pillar[n]arenes”.<sup>1,2</sup> Linear 1,2-dichloroethane and bulky chlorocyclohexane acted as template solvents for high-yield synthesis of pillar[5]- and pillar[6]arenes, respectively. They have unique symmetrical pillar structures due to their para-bridge linkage. We have synthesized various topological and functional molecules based on functionality of pillar[n]arenes, and constructed 2D sheets and 3D vesicles based on geometric assemblies of their pentagonal and hexagonal structures.<sup>3</sup>



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# Design of organo-sulfur catalysts

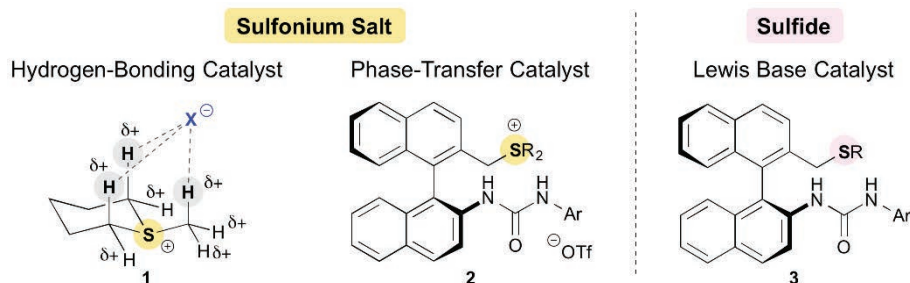
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Despite the wide synthetic utility of onium salt compounds as reagents and catalysts, the catalytic ability of tertiary sulfonium salts has not yet been demonstrated well in organic synthesis. To create new possibilities for sulfonium salts as catalysts, we focused on the hydrogen-bonding abilities of  $\alpha$  hydrogen atoms on alkylsulfonium salts when we reported the use of newly-designed tetraalkylammonium salts as hydrogen-bonding catalysts on the basis of the characteristic properties of the  $\alpha$  hydrogen atoms.<sup>1</sup> Based on the design of the tetraalkylammonium salts, we focused on simple cyclic trialkylsulfonium salts.<sup>1</sup> The catalytic ability of trialkylsulfonium salts was superior to that of the related tetraalkylammonium salts in organic reactions.<sup>2</sup>

We also have successfully demonstrated that chiral tertiary sulfonium salt catalysts can promote asymmetric reactions. Binaphthyl-modified bifunctional sulfonium salts<sup>2</sup> were efficient catalysts for the asymmetric conjugate additions under base-free neutral phase-transfer conditions.<sup>3</sup> As far as could be ascertained, this is the first example of a highly enantioselective reaction catalyzed by chiral tertiary sulfonium salts.

Based on the design of chiral sulfonium salts,<sup>2</sup> chiral sulfide catalysts<sup>3</sup> have also been synthesized and utilized as effective Lewis base catalysts.



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# Supramolecular polymeric materials functionalized by host-guest interactions and its stimuli-responsive properties

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Molecular recognition chemistry and supramolecular chemistry have received much attention, owing to their effects on catalytic activity, molecular switches, and materials. Stimuli-responsive supramolecular polymers is relevant not only for biological functions but also for a range of other applications. Our research group has employed cyclodextrins (CDs) as host molecules. In this presentation, I would like to introduce our studies to realize sol-gel switching, self-healing, adhesion control, and contraction-expansion properties through the formation of inclusion complexes with CDs (Fig. 1).

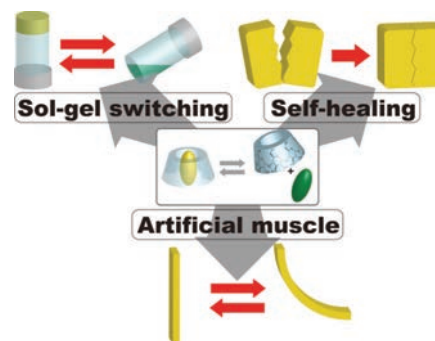
**Adhesion and self-healing material:** First, adhesion between the host hydrogel with  $\beta$ CD and the guest hydrogel with an adamantyl (Ad) group was investigated. The  $\beta$ CD hydrogel selectively adheres to the Ad guest hydrogel without mismatching (Fig. 2).

Next, we prepared effective self-healing materials based on  $\beta$ CD and Ad units. When two cut surfaces were brought into contact, the two pieces adhered. The adhered materials showed almost complete recovery of the initial material strength. The recovery ratio of the rupture strength increased with adhesive time. Interestingly, only cut surfaces showed a self-healing property, whereas uncut surfaces did not.

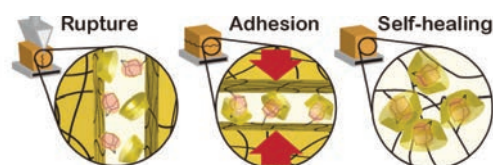
**Photoresponsive materials:** Two structural approaches may realize supramolecular actuators through host-guest interactions: a method with a linear main chain and one with a side chain in the polymer structure (Fig. 3). We have prepared photo responsive supramolecular actuators by integrating host-guest interactions on the polymer side chains (Fig. 3a). Another supramolecular hydrogels containing CD-based [c2] daisy chains as crosslinkers contract and expand through photoresponsive sliding motions of the [c2]daisy chain (Fig. 3b).

## References

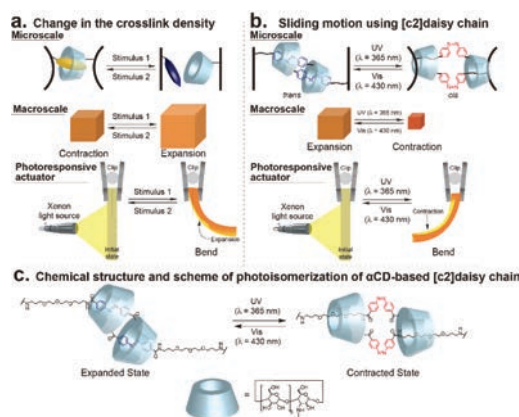
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**Figure 1.** Supramolecular materials based on host-guest interactions with cyclodextrins (CDs).



**Figure 2.** Self-healing materials based on host-guest interactions.



**Figure 3.** Supramolecular actuators using CD derivatives. The actuators show macroscopic



Notes



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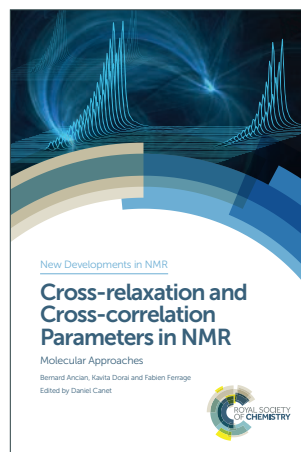
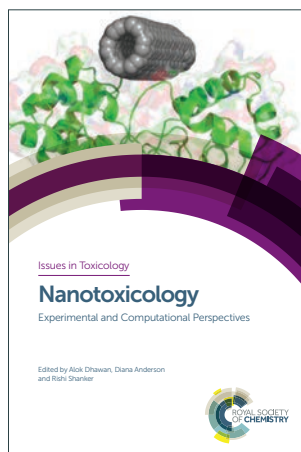
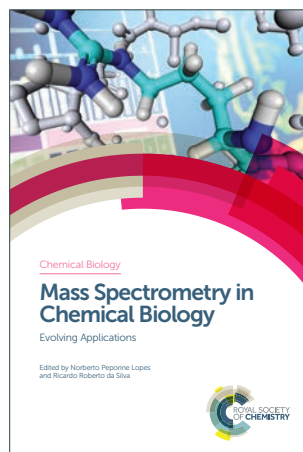
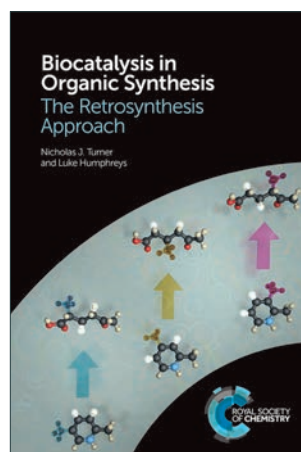
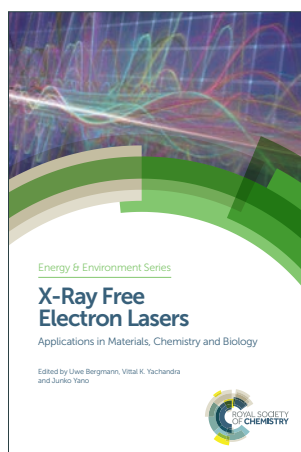
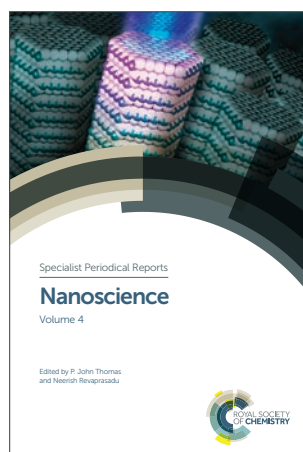
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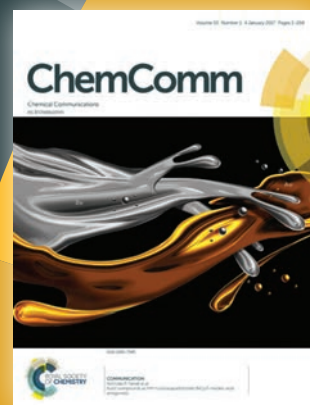
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