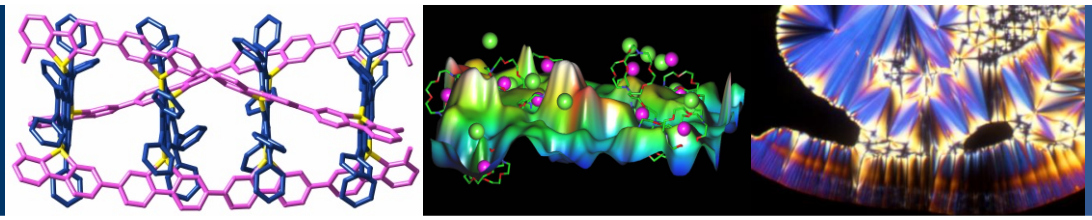
UNIVERSITÉ DE STRASBOURG

FACULTÉ DE CHIMIE STRASBOURG

Strasbourg Summer School

Challenges in Supramolecular Chemistry



from 8 to 12 September 2014,
at the Institute de Science et d'Ingénierie Supramoléculaires (ISIS),
Strasbourg, France

Supramolecular Chemistry...

initiated by Jean-Marie Lehn in Strasbourg some forty years ago, is today a central discipline in chemistry and its frontiers with physics, biology and technology. The Faculty of Chemistry of the University of Strasbourg is honored to welcome you for its first summer school entitled «Challenges in Supramolecular Chemistry».

The event takes place in Strasbourg at ISIS from 8 to 12 September 2014. The school brings together some of the most renowned international specialists of the field presenting the state of the art achievements in the area.

This school is meant to be the first step towards a close collaboration between the universities of Strasbourg, Barcelona, Bologna and Groningen in the field of teaching. Building on strong research capacities in the field, our institutions commit themselves to prepare a Master of excellence in supramolecular chemistry.

The Organization Committee

Table of Contents

Site map

How to get to the Central Campus - Esplanade ?

From the airport:

Take the airport shuttle until the terminus "Baggersee", then take the tram line E, direction "Baggersee" and get off at the stop "Observatoire".

From the train station:

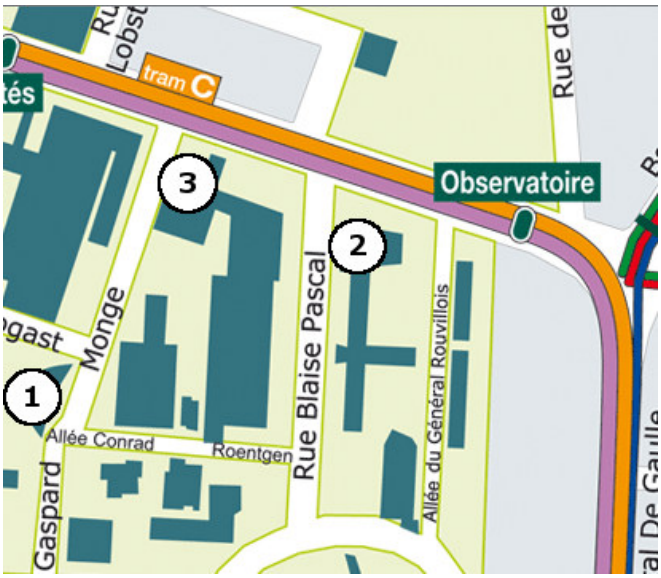
Take the tram line C, direction "Neuhof / Rodolphe Reuss" and get off at the stop "Observatoire".

Find your way at the Esplanade campus

The school will essentially take place in the main conference room of the Institut de Science et d'Ingénierie Supramoléculaires (ISIS), 8 allée Gaspard Monge (1).

Monday evening, we will invite you to a Welcome Party at the "Cafétéria" of the Chemistry Faculty, 1 rue Blaise Pascal (2).

And lunch will be offered every day at the University restaurant "Le 32", 32 boulevard de la Victoire (3).



Relevant adresses for the cultural program

Departure for the Boattrip (Wednesday evening):

The boat will start at 17:30. We will have to be there at 17:10. Adresse: Batorama, place du Marché aux Poissons

The Gala Diner (Wednesday evening):

Diner will start at 19:30 at the restaurant "Ancienne Douane", 6 rue de la Douane

From the conference site to the boat, you will need about 20 minutes by foot and/or tram. From the boat to the restaurant, you will need about ten minutes by foot.

Program

Monday, 8 Septembre

13:00 - 14:30	Registration and Coffee
14:30 - 16:00	Jean-Marie LEHN, Perspectives in Chemistry : From Molecular to Supramolecular Chemistry towards Adaptive Chemistry
16:00 - 16:30	Coffee Break
16:30 - 18:00	Jean-Marie LEHN, Perspectives in Chemistry : From Molecular to Supramolecular Chemistry towards Adaptive Chemistry
18:00 - 20:00	Welcome Party (2)

Tuesday, 9 Septembre

09:00 - 10:30	Harry ANDERSON, An introduction to Molecular Wires
10:30 - 10:45	Coffee Break
10:45 - 12:00	Harry ANDERSON, Template-Directed Synthesis of Porphyrin Nanorings
12:00 - 14:00	Lunch (3)
14:00 - 16:00	Thomas WARD, Supramolecular Anchoring Strategies for the Creation of Artificial Metalloenzymes: Challenges and Opportunities
16:00 - 16:30	Coffee Break
16:30 - 18:30	Jaume VECIANA, Supramolecular organizations as novel nanomedicines for drug delivery
18:45 - 20:30	Poster session

Wednesday, 10 Septembre

9:00 - 10:30	Jean-Pierre SAUVAGE, From Chemical Topology to Molecular Machines
10:30 - 10:45	Coffee Break
10:45 - 12:00	Jean-Pierre SAUVAGE, From Chemical Topology to Molecular Machines
12:00 - 14:00	Lunch (3)
14:00 - 15:00	Margherita VENTURI, Supramolecular Chemistry at Work: Molecular-Level Devices And Machines
15:00 - 15:15	Coffee Break

15:15 - 16:30	Margherita VENTURI, Supramolecular Chemistry at Work: Molecular-Level Devices And Machines
16:30 - 19:00	Social Program (Boat trip starts at 17:30)
19:30 - 21:30	Gala Dinner (at the restaurant "Ancienne Douane")

Thursday, 11 Septembre

9:00 - 10:30	Makoto FUJITA, Coordination Self-Assembly: From Principle to Applications
10:30 - 10:45	Coffee Break
10:45 - 12:00	Makoto FUJITA, Coordination Self-Assembly: From Principle to Applications
12:00 - 14:00	Lunch (3)
14:00 - 15:30	Mir Wais HOSSEINI, Molecular tectonics
15:30 - 15:45	Coffee Break
15:45 - 17:00	Mir Wais HOSSEINI, Molecular tectonics
17:15 - 19:00	Poster session

Friday, 12 Septembre

9:00 - 10:30	Sijbren OTTO, Supramolecular Systems Chemistry
10:30 - 10:45	Coffee Break
10:45 - 12:00	Sijbren OTTO, Supramolecular Systems Chemistry

Poster Sessions

Tuesday, 9 Septembre

P 1	Kiyohiro ADACHI	A Peptidic Four-Leaf-Clover-Like Macrocycle
P2	Yigit ALTAY	Self-Replicators from Dynamic Combinatorial Libraries
P3	Tatsuhiko ARAI	Absolute structure determination of chiral compounds by chiral porous coordination network
P4	Eline BARTOLAMI	Dynamic expression of multivalent recognition of DNA
P5	Ole BEYER	A [2]rotaxane shuttle with a fluorous ponytail for proton transport
P6	Iris BITTNER	Synthesis of Substituted Conductive Diarylethenes
P7	Romain CORSO	Porous Chiral Coordination Networks
P8	Dawei ZHANG	A fluorescent Zn(II)@hemicryptophane cage for heteroditopic recognition of phosphorylated choline
P9	Benjamin DOISTAU	Switchable Molecular Tweezers: Luminescent or Magnetic
P10	Emile ENGEL	Negative thermal expansion facilitated by weak host-guest interactions
P11	Sloane EVARISTE	Pre-assembled polymetallic precursors based on organophosphorus ligands for supramolecular assemblies
P12	Svenja FISCHMANN	A Double Selection Process for Ion Transport Using Dynamic Covalent Chemistry
P13	Matthew FREITAG	Formation of Polydiacetylenes From Higher Order Diiodopolyynes
P14	Yuya FUJII	Regioselective Spirocyclization of Biphenylacetylenes within a Hollow Cage
P15	Andreas HUSSAIN	Dynamic combinatorial libraries operated far from-equilibrium: toward dissipative molecular networks

Thursday, 11 Septembre

P16	Nicolas MARETS	Molecular tectonics based nanopatterning of interfaces with 2D metal-organic frameworks (MOFs)
P17	Antoine MAZEL	Azadipyrrin based heterometallic coordination networks
P18	Luis MOREIRA NAVARRO	Unveiling the nature of supramolecular crown ether-C60 interactions
P19	Takafumi OSUGA	Three-dimensional Au(I) arrays on a tray-shaped Au3 scaffold
P20	Tobias OTREMBA	Linear and Cyclic Peptide based Boronic Acid functionalized Carbohydrate Receptors
P21	Jérémy SCELLE	Functionalized Cyclodextrin Polyrotaxanes for Bimodal Imaging
P22	Manuel SOUTO	Self-assembled architectures with segregated donor and acceptor units of a new monopyrrolo-TTF-PTM radical
P23	Yuki TAKAHASHI	X-ray Crystallographic Analysis of Organometallic Compounds Using Crystalline Sponge Method
P24	Meniz TEZCAN	Towards Speciation in Self-Replicating Systems Containing Mutated Building Blocks
P25	Arnaud TRON	LIGHT-DRIVEN HYDROGEN-BONDED [2]ROTAXANE FORMATION
P26	Yoshihiro UEDA	Self-Assembly of M30L60 Icosidodecahedron
P27	Elena VULPE	Molecular tectonics: fluorinated porphyrin based coordination networks
P28	Shitao WANG	A Self-Assembled M3nLn Coordination Capsule with Large Structural Change for Guest Encapsulation
P29	Chaojie XU	Synthesis of Chiral Iridium complexes for the formation of Coordination networks

LECTURES

Perspectives in Chemistry: From Molecular to Supramolecular Chemistry towards Adaptive Chemistry

Jean-Marie LEHN (lehn@unistra.fr)
ISIS, Université de Strasbourg

Chemistry is the science of the structure and transformation of non-living and living matter. It plays a basic role in the path towards understanding how matter has become complex, from the atom to the thinking organism in the course of the evolution of the universe.

Molecular chemistry has developed a wide range of very powerful procedures for mastering the organisation of matter and building ever more complicated molecules from atoms linked by covalent bonds.

Supramolecular chemistry lies beyond molecular chemistry. It aims at constructing and implementing highly complex chemical systems from molecular components held together by non-covalent intermolecular forces. It has relied on the development of preorganized molecular receptors for effecting molecular recognition, catalysis and transport processes, on the basis of the molecular information stored in the covalent framework of the components and read out at the supramolecular level through specific interactional algorithms. It has explored the design of functional

A further step consists in the design of systems undergoing self-organization, i.e. systems capable of spontaneously generating well-defined functional supramolecular architectures by self-assembly from their components, on the basis of the molecular information stored in the covalent framework of the components and read out at the supramolecular level through specific non-covalent interactional algorithms, thus behaving as programmed chemical systems. Chemistry may therefore also be considered as an information science, the science of informed matter.

The design of molecular information controlled, “programmed” and functional self-organizing systems provides an original approach to nanoscience and nanotechnology. It represents a means of performing programmed engineering and processing of functional nanostructures. It offers a very powerful complement or alternative to nanofabrication.

Supramolecular chemistry is intrinsically a dynamic chemistry in view of the lability of the interactions connecting the molecular components of a supramolecular entity and the resulting ability of supramolecular species to exchange their constituents. The same holds for molecular chemistry when the molecular entity contains covalent bonds that may form and break reversibility, so as to allow a continuous change in constitution by reorganization and exchange of building blocks. These features define a Constitutional Dynamic Chemistry (CDC) on both the molecular and supramolecular levels.

CDC introduces a paradigm shift with respect to constitutionally static chemistry. The latter relies on design for the generation of a target entity, whereas CDC takes advantage of dynamic diversity to allow variation and selection. The implementation of selection in chemistry introduces a fundamental change in outlook. Whereas self-organization by design strives to achieve full control over the output molecular or supramolecular entity by explicit programming, self-organization with selection operates on dynamic constitutional diversity in response to either internal or external factors to achieve adaptation.

In the process of reaching higher levels of self-organisation, CDC gives access to the generation of networks of dynamically interconverting constituents connected either structurally (molecular and supramolecular arrays) or reactionnally (set of connected reactions) or both. They define a class of constitutional dynamic networks (CDNs), presenting agonistic and antagonistic relationships between their constituents, that may couple to thermodynamic or kinetic processes and respond to perturbations by physical stimuli or to chemical effectors.

The merging of the features: - information and programmability, - dynamics and reversibility, -constitution and structural diversity, opens vast perspectives and points towards the emergence of adaptive and evolutive chemistry on the way towards systems of increasing complexity.

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Lehn, J.-M., Perspectives in Chemistry – Steps towards Complex Matter, Angew. Chem. Int. Ed., 2013, 52, 2836-2850.

Lehn, J.-M., Dynamers : From Supramolecular Polymers to Adaptive Dynamic Polymers, Adv. Polym. Sci., 2013, 261, 155-172.

Lecture 1: An introduction to Molecular Wires

Lecture 2: Template-Directed Synthesis of Porphyrin Nanorings

Harry L. Anderson (harry.anderson@chem.ox.ac.uk)
Department of Chemistry, University of Oxford

Lecture 1:

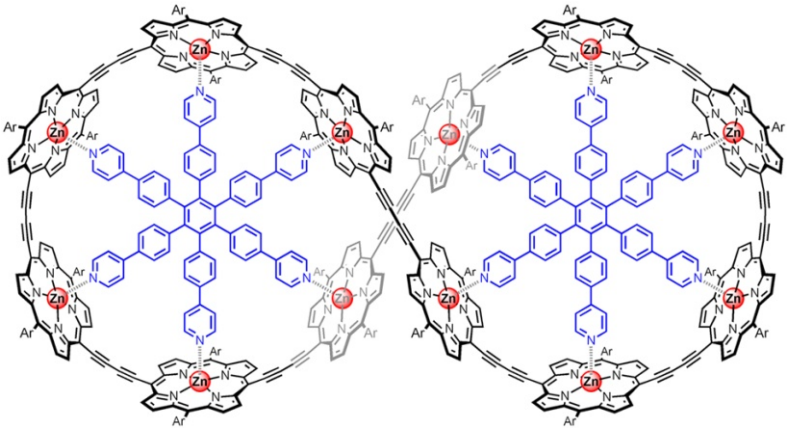
An introduction to Molecular Wires

This lecture will provide an introductory overview of the chemistry and physics of molecular wires, to address questions such as: How can we design a molecule to mediate charge transport? How can we measure the conductance of a single molecule?

Lecture 2:

Template-Directed Synthesis of Porphyrin Nanorings

Conjugated porphyrin oligomers exhibit remarkable properties, including wire-like charge transport, ultrafast energy migration, nonlinear refraction and strong two-photon absorption. They are amazingly amenable to supramolecular control, and the coordination chemistry of the metal centers leads wide possibilities for template-directed synthesis. This lecture will provide an introduction to template-directed synthesis, and show how simple strategies can be devised to synthesize π-conjugated nanorings which enter the size domain of a typical protein, such as the figure-of-eight complex shown below.[1]



[1] M. C. O'Sullivan, J. K. Sprafke, D. V. Kondratuk, C. Rinfray, T. D. W. Claridge, A. Saywell, M. O. Blunt, J. N. O'Shea, P. H. Beton, M. Malfois, H. L. Anderson, Nature 2011, 469, 72–75.

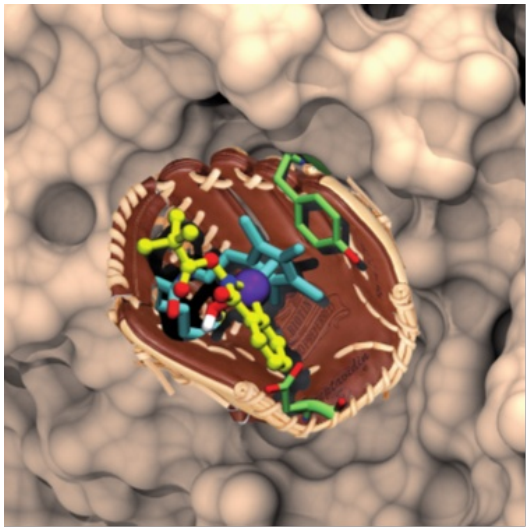
Supramolecular Anchoring Strategies for the Creation of Artificial Metalloenzymes: Challenges and Opportunities

Thomas R. Ward (thomas.ward@unibas.ch)
University of Basel

Artificial metalloenzymes result from incorporation of a catalytically competent organometallic moiety within a host protein. We and others have been exploiting the potential of the biotin-(strept)avidin tech-nology for the creation of artificial metalloenzymes, Figure. Thanks to the remarkable supramolecular affinity of biotin for either avidin or streptavidin (KD > 10-13 M), linking of a biotin anchor to a catalyst precursor ensures that, upon stoichiometric addition of (strept)avidin, the metal moiety is quantitatively incorporated within the host protein.

Such supromolecular artificial metalloen-zymes are optimized either by chemical (variation of the biotin-spacer-ligand moiety) or genetic-(mutation of (strept)avidin) means. These chemogene-tic schemes were applied to optimize the performance for eight different catalyzed transformations as well reaction cascades in the presence of natural enzymes.[1-3]

More recently, we have been exploiting the tetrameric nature of streptavidin to fine-tune the performance of such supramolecular catalysts for a variety of transformations. In this context recent progress, challenges and opportunities will be presented.



Reactions implemented thus far:
Hydrogenation (up to 96 % ee)
Transfer Hydrogenation of ketones (up to 98 % ee)
imines (up to 96 % ee)
enones (up to 1000 TONs)
Allylic Alkylation (up to 95% ee)
C-H Activation (up to 86 % ee)
Olefin Metathesis (up to 40 TONs)
Alcohol Oxidation (up to 250 TONs)
Sulfoxidation (up to 93 % ee)
Dihydroxylation (up to 98 % ee)

Figure. Artificial metalloenzymes obtained upon supramolecular incorporation of a biotinylated organometallic catalyst within streptavidin

1. Ward, T. R. Acc Chem Res 44, 47–57 (2011).
2. Köhler, V. et al. Nature Chem 5, 93–99 (2012).
3. Hyster, T. K., Knorr, L., Ward, T. R. & Rovis, T. Science 338, 500–503 (2012).

Supramolecular organizations as novel nanomedicines for drug delivery

Jaume Veciana (vecianaj@icmab.es)
CSIC and CIBER-BBN, Bellaterra

The objective of this lecture is to give a broad overview of how nanotechnology is impacting in some areas of medicine and pharmacology. Brief basic concepts in nanomedicine and biomaterials will be detailed at the beginning of the lecture. Following the introduction, the lecture will report the advantages of nanoparticulate molecule-based organizations for drug delivery and clinical diagnosis. It has been reported that polymeric nanoparticles and nanovesicles are efficient drug carriers that can significantly help to develop new drug delivery routes, and more selective and efficient drugs with a higher permeability to biological membranes and with controlled released profiles, as well as to enhance their targeting towards particular tissues or cells [1-2].

The potential of nanotechnology «bottom-up» strategies, based on molecular self-assembling, is much larger than that of «top-down» approaches for the preparation of such nanosized supramolecular organizations. For instance, by precipitation procedures it should be possible to control particle size and size distribution, morphology and particle supramolecular structure. However, conventional methods from liquid solutions have serious limitations and are not adequate for producing such nanoparticulate materials at large scale with the narrow structural variability, high reproducibility, purity and cost needed to satisfy the high-performance requirements and regulatory demands dictated by the USA and European medicine agencies. On the contrary, using compressed solvent media it is possible to obtain supramolecular materials with unique physicochemical characteristics (size, porosity, polymorphic nature morphology, molecular self-assembling, etc.) unachievable with classical liquid media. The most widely used CF is CO2, which has gained considerable attention, during the past few years as a «green substitute» to organic solvents. Due to such properties, during the past few years CFs based technologies are attracting increasing interest for the preparation of nanoparticles and nanovesicles with application in nanomedicine.

In this lecture a simple one-step and scale-up methodology for preparing multifunctional nanovesicle-drug conjugates will be presented. This method is readily amenable to the integration/encapsulation of multiple bioactive components, like peptides, proteins, enzymes, into the vesicles in a single-step yielding sufficient quantities for clinical research becoming, thereby, nanocarriers to be used in nanomedicine. A couple of examples of novel nanomedicines for solving serious diseases, prepared by this methodology, will be presented and their advantages discussed [3-4].

References

[1] M. E. Davis, Z. Chen, D. M. Shin, Nature Reviews-Drug Discovery 2008, 7, 771-782. [2] J. A. Hubbell, R. Langer, Nature Materials, 2013, 12, 963-966. [3] N. Ventosa, L. Ferrer-Tasies, E. Moreno-Calvo, M. Cano, M. Aguilella, A. Angelova, S. Lesieur, S. Ricart, J. Faraudo, J. Veciana. Langmuir, 2013, 29, 6519-6528. [4] I. Cabrera, E. Elizondo, E. Olga; J. Corchero, M. Mergarejo, D. Pulido, A. Cordoba, E. Moreno-Calvo, U. Unzueta, E. Vazquez, I. Abasolo, S. Schwartz, A. Villaverde, F. Albericio, M. Royo, M. Garcia, N. Ventosa, J. Veciana. Nano Letters, 2013, 13, 3766-3774.

From Chemical Topology to Molecular Machines

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ISIS, Université de Strasbourg

Two distinct but related topics will be considered, in relation to the historical context of the various approaches discussed during the lectures. In addition, some of the most recent and significant contributions reported by various research groups working in the fields will be described.

1. Chemical Topology[1]

This area is mostly concerned with molecules whose molecular graph is non planar, i.e. which can not be represented in a plane without crossing points. The most important family of such compounds is that of catenanes and rotaxanes. The simplest catenane, a [2]catenane, consists of two interlocking rings. Rotaxanes consist of rings threaded by acyclic fragments (axes). The simplest rotaxane, a [2]rotaxane, contains two non-covalently connected components : a ring and an axis, the axis being end-functionalised by bulky groups preventing unthreading of the non cyclic fragment from the cycle. Interlocking ring compounds (also named "Mechanically Interlocked Molecules") have attracted much interest in the molecular sciences, first as pure synthetic challenges and, more recently, as components of functional materials. The synthesis of such compounds relies on templates (transition metals or organic assemblies). In recent years, spectacular progress has been made. Highly functional and complex systems have been reported by several research teams, demonstrating the power of modern synthetic tools based on "template effects".

2. Molecular Machines[2]

Separately, the field of artificial molecular machines has experienced a spectacular development, in relation to molecular devices at the nanometric level or mimics of biological motors. In biology, motor proteins are of the utmost importance in a large variety of processes essential to life (ATPase, a rotary motor, or the myosin-actin complex of striated muscles behaving as a linear motor responsible for contraction or elongation). A few recent examples are based on simple or more complex rotaxanes or catenanes acting as switchable systems or molecular machines. Particularly significant examples include "molecular shuttles" as well as multi-rotaxanes reminiscent of muscles or able to act as switchable receptors. Some of the machine-like compounds have been deposited on surfaces or incorporated in mesophase. The molecules are set in motion using electrochemical, photonic or chemical signals. Examples will be given which cover the various approaches used for triggering the molecular motions implied in the synthetic molecular machine prototypes recently reported.

References

1. R.S. Forgan, J.-P. Sauvage & J.F. Stoddart, Chem. Rev., 2011, 111, 5434-5464.
2. a) V. Balzani, A. Credi, M. Venturi, "Molecular Devices and Machines – Concepts and Perspectives for the Nanoworld", Wiley-VCH, 2008. b) "From Non-Covalent Assemblies to Molecular Machines", J.-P. Sauvage & P. Gaspard Ed., Wiley-VCH, 2011.

SUPRAMOLECULAR CHEMISTRY AT WORK: MOLECULAR-LEVEL DEVICES AND MACHINES

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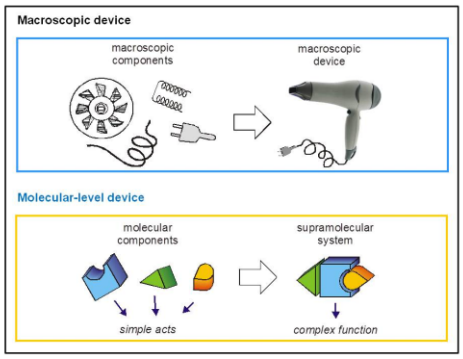
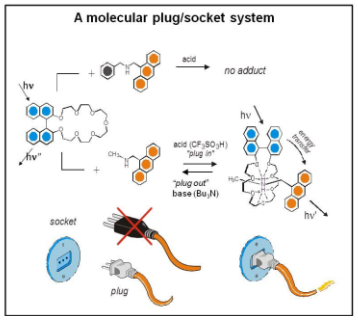
DIPARTIMENTO "G. CIAMICIAN", UNIVERSITÀ DI BOLOGNA

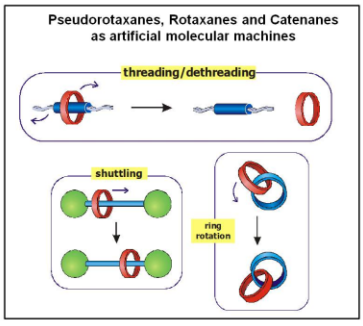
Supramolecular (multicomponent) systems can perform complex functions which result from the cooperation of actions performed by suitably selected molecular components. Looking at supramolecular systems from the viewpoint of the functions shows that the concept of macroscopic device can be extended to molecular level.



Of particular interest are molecular-scale devices in which the component parts are capable of performing mechanical-like movements as a consequence of an appropriate energy supply, that is, molecular machines. Nature exploits very complex molecular-level devices and machines to sustain life, and, in the last thirty years, the development of Supramolecular Chemistry has allowed the construction of simple molecular-level devices and machines, that are important not only for basic research, but also for the growth of nanotechnology.

Molecular devices and machines are chemical systems and, therefore, they operate by means of chemical reactions that, broadly speaking, imply both electronic and nuclear rearrangements. In some cases, however, the function performed is essentially based on the transfer of electrons or electronic energy, whereas in other cases, the operation is based on the occurrence of more or less extensive nuclear displacements caused by electronic rearrangements.





As it happens in the macroscopic world, molecular-level devices and machines need energy to operate and signals to communicate with the operator.

The energy needed for the operation of a molecular device or machine can be supplied in the form of (i) a chemical reagent, (ii) an absorbed photon, or (iii) addition or subtraction of an electron.

Examples of artificial molecular-level devices and machines investigated in our laboratory will be discussed.

References:

To read more: V. Balzani, A. Credi, M. Venturi, Molecular Devices and Machines – Concepts and Perspectives for the Nanoworld, 2nd Edition, Wiley-VCH, Weinheim, 2008.

Coordination Self-Assembly: from Principle to Applications

Makoto Fujita (mfujita@appchem.t.u-tokyo.ac.jp)
Department of Applied Chemistry, The University of Tokyo

Lecture I: Structure and Function on the Nanoscale

Molecular self-assembly based on coordination chemistry has made an explosive development in recent years. Over the last two decades, we have been showing that the simple combination of transition-metal's square planer geometry (a 90 degree coordination angle) with pyridine-based bridging ligands gives rise to the quantitative self-assembly of nano-sized, discrete organic frameworks. Representative examples include square molecules *(JACS 1990)*, linked-ring molecules *(Nature 1994 & 1999)*, cages *(Nature 1995)*, tubes *(JACS 2004)*, and capsules *(Nature 1999)* that are self-assembled from simple and small components. Following the discussion on the structures of coordination assemblies, focus will be on the cavity-directed reaction and property control of organic molecules, which represent one of the most important features of three-dimentional hosts (see review: *Angew. Chem. IE. 2009, 48, 3418*). Furthermore, the powerful technique of coordination self-assembly has been applied to the bottom-up construction of discrete, well-defined nano-scale structures. Large (> 50) multi-component systems offer not only structural but also mechanistic insights into biological assembly. The self-assembly of giant, MnL2n coordination spheres from n palladium ions (M) and 2n curved bridging ligands (L) will be focused. The structure of these multi-component systems is highly sensitive to the geometry of the bent ligands. Even a slight change in the ligand bend angle critically switches the final structure observed across the entire ensemble of building blocks between M24L48 and M12L24 coordination spheres (Science 2010). Functionalization at the periphery and the interior of the giant spheres will be also discussed.

Lecture II Crystal-Free Crystallography

X-ray single crystal diffraction (SCD) analysis has the intrinsic limitation that the target molecules must be obtained as single crystals. In this talk, a new protocol for SCD analysis that does not require the crystallization of the sample. In our method, tiny crystals of porous complexes are soaked in the solution of a target, where the complexes can absorb the target molecules. The crystallographic analysis clearly determines the absorbed guest structures along with the host frameworks. As the SCD analysis is carried out with only one tiny crystal, the required sample amount is of the nano-to-microgram order. With chiral guests, the space group of the crystal turned into chiral (C2 or P1), enabling the determination of absolute configuration of the guests from the anomalous scattering from the host ZnI2 component. We demonstrate that even ~50 ng of a sample is enough to be analyzed. When combined with high performance liquid chromatography (HPLC), multiple fractions were directly characterized, establishing a prototypical LC-SCD analysis. Detailed protocols for our method will be soon published. Major references are: *JACS 1994, 116, 1151; Nat. Chem. 2010, 2,780; Angew. Chem. IE 2012, 51, 2379; JACS 2011, 133, 19691; JACS 2011, 133, 16806; Nature, 2013, 495, 461.*

Molecular tectonics

Mir Wais Hosseini (hosseini@unistra.fr)

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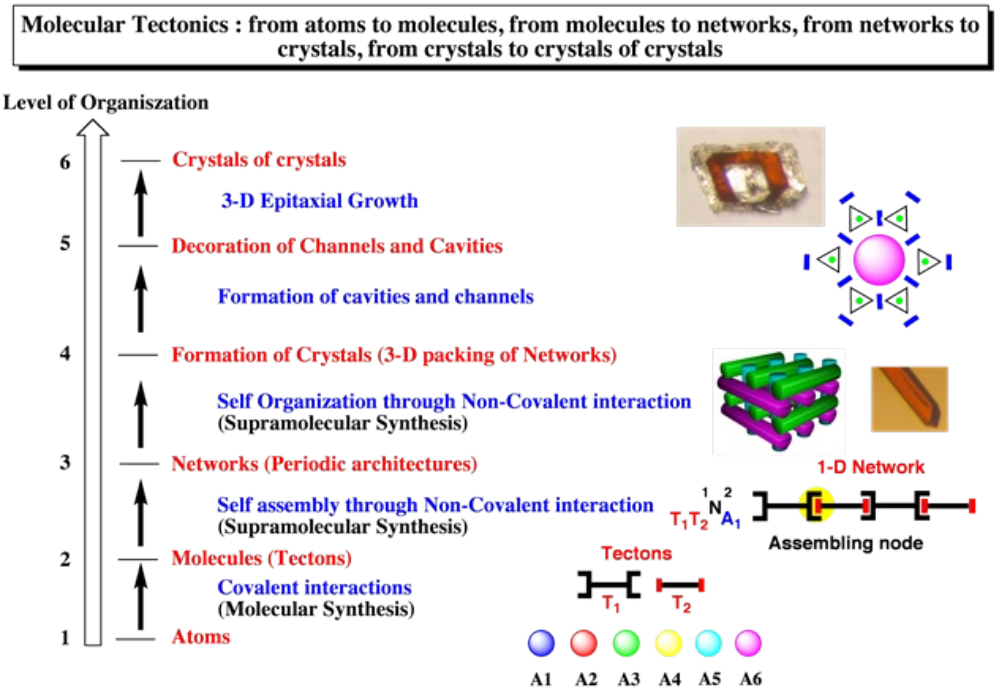
The design and construction of periodic architectures in the crystalline phase are attracting considerable interest over the last two decades. Molecular tectonics is a versatile approach for the design, analysis and description of molecular crystals. This approach, based on the formation of molecular networks by complementary tectons or construction units in the solid state, combines molecular and supramolecular syntheses. The generation of molecular networks and subsequently of crystals is achieved by self-assembly processes through repetitive molecular recognition events. The lecture will present general principles of molecular tectonics such as formal definition of tectons (denticity, hapticity) and their mutual recognition (mode and energy of intermolecular interactions), networks both in terms of topology (connectivity patterns and dimensionality), geometry (shape), packing, interpenetration and directionality. The concepts will be illustrated by a variety of tectons, networks and complex purely organic or hybrid architectures. Finally, the versatility of principles developed in molecular tectonics will be demonstrated through the design and hierarchical construction of crystals of crystals by 3D epitaxial growth.



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Supramolecular Systems Chemistry

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Supramolecular chemistry provides a powerful entry into the emerging field of systems chemistry, which may be loosely defined as the study of mixtures of interacting molecules that show emergent properties. Emergent properties are characteristics of a system that arise from the system as a whole and that cannot be ascribed to any of the components acting in isolation.

The lecture will start with focussing on supramolecular systems under thermodynamic control, where the products are determined by the lowest free energy state of the system. Where supramolecular chemistry started by focusing on relatively simple systems, attention is now increasingly shifting to more complex mixtures. This trend has given rise to the field of dynamic combinatorial chemistry which are mixtures of interconverting molecules at equilibrium. Dynamic combinatorial libraries have become useful tools for the development of synthetic receptors and ligands for biomolecules, and more recently also for discovering new self-replicating molecules and self-synthesizing materials. They also show some perhaps counterintuitive systems behaviour.

Where supramolecular systems under thermodynamic control are relatively predictable they are also somewhat limited. At any given set of conditions the system can only be in a single state: the thermodynamic minimum. In contrast, when systems are under kinetic control, different states may be reached, depending on the pathway that was followed when preparing the system. Hence kinetically controlled systems are potentially more versatile than thermodynamically controlled ones, but also much more difficult to control. Notwithstanding, the development of kinetically controlled self-assembling systems is now becoming increasingly popular as will be illustrated with some examples.

An even more versatile thermodynamic regime involves systems that are far from equilibrium. For such systems a continuous energy supply is needed to sustain them; i.e. dissipate energy. By tapping into this energy supply far-from-equilibrium systems can have unique functions, that are not possible under kinetic or thermodynamic control. Life is a prime example of a self-organized system that is far from equilibrium. Other emergent behaviour include: dissipative self-assembly, unidirectional rotation and oscillations. Very recently supramolecular chemists have started to design systems that operate in this thermodynamic regime. Some leading examples will illustrate this development.

Poster Abstracts

P1

A Peptidic Four-Leaf-Clover-Like Macrocycle

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Incorporation of d-amino acid residues (D) into l-peptides (l-amino acid: L) can afford unique curved conformations. For example, gramicidin A and polytheonamide B, natural bacterial peptides, have unique β-helical structures based on their L-D alternating sequences.1 In addition, artificially-cyclized peptides of such L-D alternating sequences adopt β-sheet macrocycles that can further form H-bonded nanotubes.2 Inspired by such an intrinsic conformational preference of curve-forming d-residues, we designed a unique peptidic macrocycle with L-D-L-L periodic sequences. Here, we report a cyclic (L-D-L-L)4 peptide, which could adopt a unique four-leaf-clover-shaped conformation (Figure 1). We expect this design enables not only the enlargement of the peptidic macrocycle but inner-functionalization with four side chains, which differs from previous (L-D)n peptides.

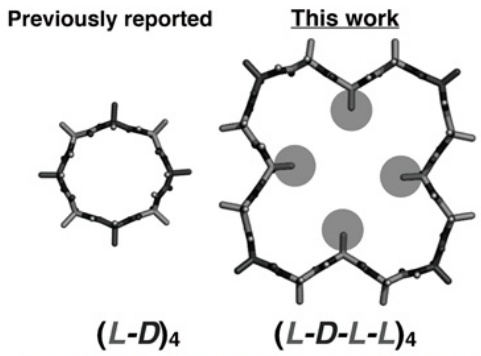

Figure 1. Previous cyclic (***L*-*D***)$_4$ peptide (*left*) and the (***L*-*D*-*L*-*L***)$_4$ cyclic peptide reported here (*right*).

L-D-L-L periodically sequenced hexadecapeptide H-(ThrBzl-d-TyrBzl-ThrBzl-Val)4-OH (1) was synthesized by liquid-phase peptide synthesis using Boc protecting group (Bzl: protecting group of side chains). Then cyclo[-(ThrBzl-d-TyrBzl-ThrBzl-Val)4-] (2) was obtained from cyclization reaction in highly dilute condition. The macrocycle 2 was efficiently obtained (183 mg, 7% total yield for 14 steps), and characterized by MALDI-TOF-MS and NMR measurements. We then examined the conformation of 2. The crystal structure of an analogous fragment, Boc-ThrBzl-d-Phe-ThrBzl-Val-OMe (3) clearly revealed the curved β-sheet conformation (Figure 2). As expected, the curve was generated around d-Phe and isopropyl group of l-Val projected inside the curve. Thus, we successfully synthesized and revealed the intrinsic propensity of L-D-L-L periodic peptides.

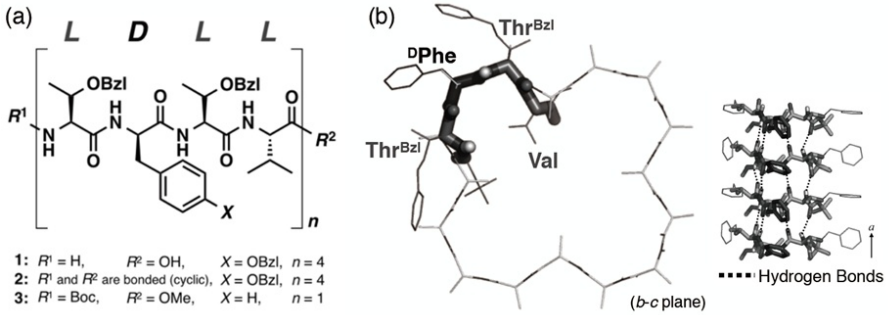

Figure 2. (a) (***L*-*D*-*L*-*L***)$_n$ periodic sequence
(b) Conformation of (***L*-*D*-*L*-*L***)$_n$ peptides (**stick**: crystal structure of **3**, **line**: proposed structure of **2**).

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P2

Self-Replicators from Dynamic Combinatorial Libraries

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One of the most fundamental questions at the interface between biology and chemistry is what constitutes the minimal molecular basis of life. There is a big gap in our knowledge considering the early steps of the formation of evolvable life. Systems chemistry, and dynamic combinatorial chemistry in particular, is a promising approach to address this intriguing question.

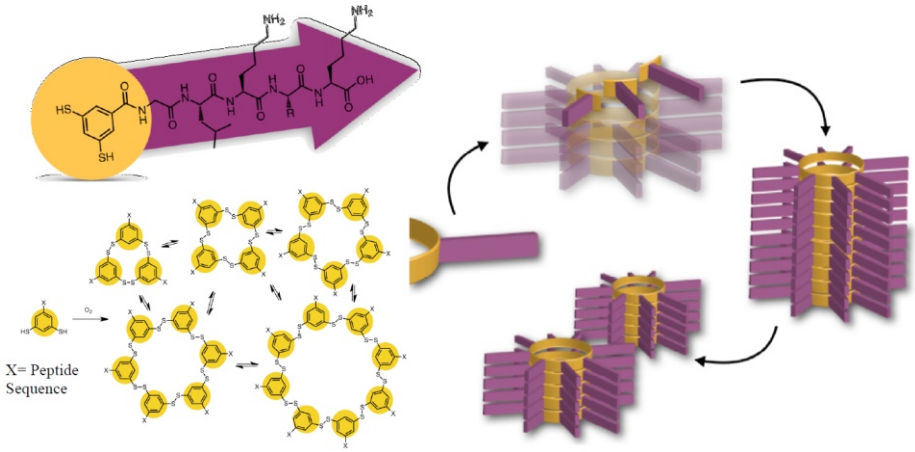

Figure 1. Schematic representation of self-replication in a dynamic combinatorial library. Building blocks form macrocycles that are under thermodynamic equilibrium with each other. When one of the macrocycles in such a network stabilise copies of itself through intermolecular non-covalent interactions, it can form fibres.The fibres can break under mechanical agitation resulting exact copies of themselves. Elongation continues on available fibre ends and this self-replication cycle can continue until all the available building blocks are used.

Self-replicating systems constructed by β-sheet prone peptide building blocks, reported up to day, formed hexamer and heptamer as the largest macrocycle size.1 The recent study of Malakoutikhah et al.2 showed that decreasing the hydrophobicity of the building blocks leads to formation of larger macrocycles consisting up to 8 building blocks. The présent aims to further extend the set of building blocks that can give rise to novel replicators. Among many parameters, the effect of changing hydrophilicity of an amino acid in the peptide sequence was chosen to explore its impact on the nature of the self-replication that emerge. If the β-sheet type interactions between the building blocks are weakened, macrocycles having a larger number of building blocks should be favoured to compensate this effect. Thus relatively hydrophilic amino acids Asn, Thr and Gly were incorporated. Furthermore, modified peptide building blocks were synthesized by introducing an amide functionality at the C-terminus. The resulting new sequences were synthesized and the replication behaviour of the dynamic combinatorial libraries made from these building blocks has been investigated.

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P3

Absolute structure determination of chiral compounds by chiral porous coordination network

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We have recently reported X-ray analysis method without crystallization process of the compounds by using the porous coordination network crystals (crystalline sponge) including the compounds.[1] The absolute structure of the chiral guest compound can be determined in this method using the distortion of the host framework by strong host-guest interaction and the anomalous scattering of heavy atoms in the framework. However, in the case of weak interaction, the absolute structure of guests cannot be determined between host and guests because of insufficient distortion of the host framework. In this work, novel crystalline sponge whose framework was originally chiral was synthesized by installing of the chiral units to the framework. Absolute structure determination of the chiral guests in the pores of the chiral crystalline sponge was achieved effectively.

The chiral crystalline sponge 1 was prepared in 34% yield by complexation of tri(4-pyridyl)-triazine (TPT) and ZnI2 with chiral aryl dioxolane 2 in nitrobenzene-methanol. The X-ray analysis of the crystal 1 revealed that 2 were installed in the framework of the crystalline sponge as the chiral units and space group of 1 is chiral P212121 (Figure 1(a)).

Inclusion of (–)-menthone 3 as the guest molecule into the crystal 1 was carried out by immersion of the crystal 1 into enantiopure 3 for 1 week at room temperature. X-ray analysis of the crystal gave the X-ray structure of 3 as 1R, 4S configuration included in the pores of the crystal (Figure 1(b)). Absolute structure of the guest molecule was successfully determined by the chiral crystalline sponge.

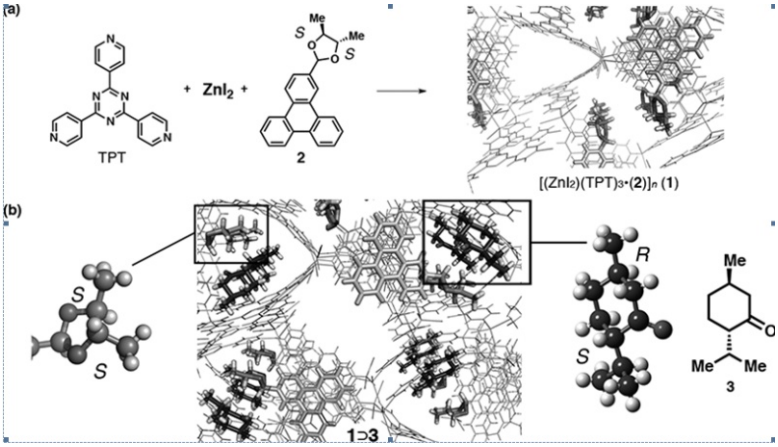

Figure 1 (a) Synthesis of chiral crystalline sponge 1 and X-ray structure. (b) X-ray structure of 3 included in the crystal 1.

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P4

Dynamic expression of multivalent recognition of DNA

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Multivalency is of great importance for the non-covalent recognition of biomolecules in aqueous media. Multivalency can emerge in situ through programmed or templated self-assembly processes.[1] In particular, reversible chemoselective and bio-orthogonal ligation techniques can be exploited for generating multivalent recognition systems through dynamic covalent chemistry.[2] For instance, we recently reported the design of dynamic materials that display a multivalent interaction with DNA and a pH-controlled degradation.[3]

Multivalent cationic clusters have recently emerged as a novel class of artificial vector for gene delivery applications.[4] Therefore, we investigated the self-assembly of biomolecular clusters through multiple acylhydrazone ligations. We selected hydrazide building blocks derived from amino acids and a pre-organized cyclodecapeptide scaffold as a "multivalency inducer". Upon mixing in aqueous media, RP-HPLC and MALDI-TOF analyses indicate the formation of the tetra-functionalized cluster. DNA recognition was then studied by a fluorescent displacement assay. While the hydrazide building blocks and the cyclodecapeptide scaffold are found to be ineffective for DNA complexation, the mixture of cationic hydrazide with the multivalency inducer display a high activity that emerge from the in situ generation of a cationic cluster through a process operated by hydrazone ligation. Furthermore, these dynamic clusters are found to undergo component exchange. The addition of methoxyamine results in the complete dissociation of the active cationic cluster and trigger the release of DNA (Figure 1). These results show that dynamic covalent chemistry can be used to manipulate in situ the expression of multivalent recognition in a controlled fashion.

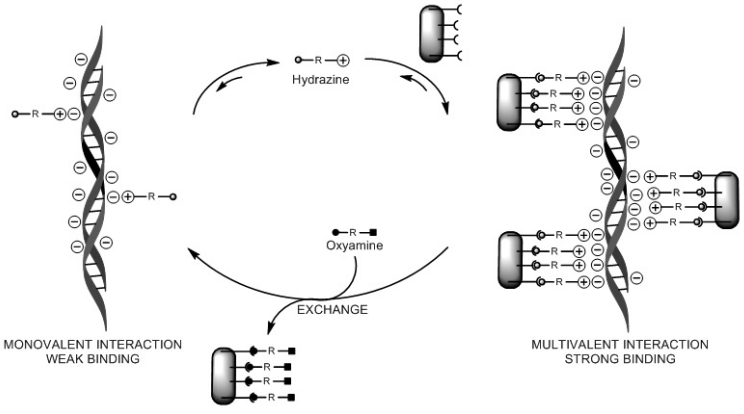

Figure 1: Dynamic generation of clusters for multivalent DNA recognition

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[2](a) Ulrich, S.; Dumy, P. Chem. Commun. 50 (2014) 5810 - 5825; (b) Corbett, P.T.; Leclaire, J.; Vial, L.; West K.R.; Wietor, J-L.; Sanders, J.K.M.; Otto, S. Chem. Rev. 106 (2006) 3652 - 3711.

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P5

A [2]rotaxane shuttle with a fluorous ponytail for proton transport

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For the development of light-driven proton pumps, several [2]rotaxane shuttles carrying a pyridine macrocycle as a ring were designed and synthesized.[1] By protonation, a Coulomb repulsion between the positive charge of the protonated pyridine and an implemented positive charge in the axis leads to a movement of the protonated pyridine macrocycle. This means, the position of the pyridine macrocycle depends on the pH value. The first [2]rotaxanes were obtained in only low yields because of synthetic and purification problems. While the synthetic problems could be solved by using an excess of the costly educts, the purification problem remains because of the similar behavior of the [2]rotaxane and free axis.

Fluorous solid phase extraction (FSPE) is a well-known method to separate fluorous compounds from each other or from non-fluorous compounds.[2] By introducing a fluorous ponytail into the ring of a [2]rotaxane, a separation of the fluorous [2]rotaxane and the non-fluorous free axis on fluorous silica gel should be possible.

Therefore, a pyridine macrocycle with a fluorous ponytail was synthesized. The fluorous [2]rotaxane was obtained by trapping the fluorous pyridine macrocycle via copper catalyzed “click” reaction of an azide halfaxis and an alkyne halfaxis (figure 1). Variation of the pH showed similar behavior for the fluorous and the related non-fluorous [2]rotaxanes, which means it can be used for proton transport. Due to the fluorous group at the macrocycle, a different elution behavior of fluorous [2]rotaxane and free axis could be observed on fluorous silica gel.

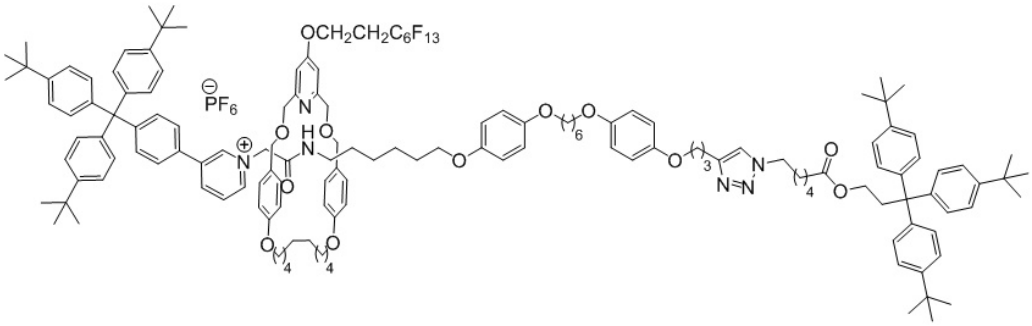

Figure 1: Fluorous [2]rotaxane for proton transport.

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P6

Synthesis of Substituted Conductive Diarylethenes

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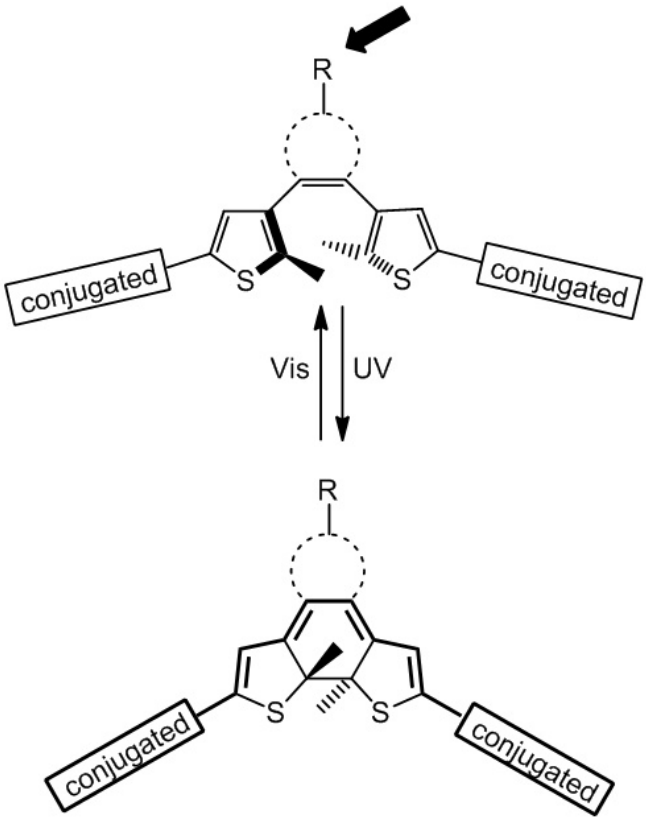
Diarylethenes which contain five-membered heterocyclic rings are well known as photochromic compounds that are thermo-irreversible, have high sensitivity and fatigue resistance properties.

In contrast to the open twisted form, the π-system is completely conjugated in the closed isomer. The result is a decrease of the HOMO-LUMO gap and consequently the increase of conductivity by the molecule.



To investigate the effect of conductance switching on surfaces without disturbing the π-system, the surface can be connected to the ethene segment. Therefore, suitable substituents have to be introduced into the central ring of the diarylethene.

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P7

Porous Chiral Coordination Networks

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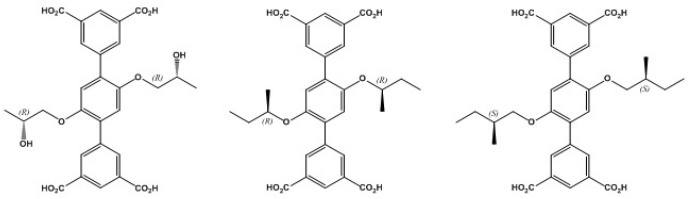
For several years now, the interest in coordination networks or metal-organic frameworks (MOFs) has been increasingdue to their structural features (dimension, topology) and their proprieties. Coordination networks are composed of organic tectons and metal centres as connecting nodes. The design, formation and description of this type of periodic architectures are subjects of the approach called Molecular Tectonics.[1, 2]

The design and generation of chiral coordination networks displaying chiral cavities and channels are of prime importance for enantiomeric and diastereoisomeric separation and/or catalysis. Using enantiomerically pure tectons bearing different chiral alkoxy-substituents, a series of isostructural porous MOFs has been synthesized and characterized.[3]

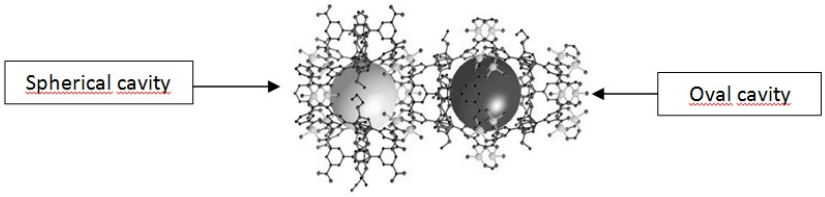
Here, we report on the use of three enantiomerically pure tectons bearing four carboxylate moieties (see bellow) and their use in the formation of chiral and robust coordination networks.



The coordination polymers obtained were structurally characterised by X-Ray diffraction on single crystals as well as by X-ray powder diffraction. All three cases studied are isostructural and display two different types of cavities, one of the oval and the other of the spherical types.

The stability of the 3D networks has been studied by thermogravimetric analysis and the phase purity established by PXRD by comparison of the experimentally determined powder X-Ray Diffraction patterns with the one simulated using the single crystal data.

The crystalline phases exhibit high permanent porosity with a Brunauer-Emmett-Teller (BET) surface area of 3831 m2 g-1and the pore volume of 1.482 cm3 g-1 after activation. These characteristics make theme promising material for gas storage and for chiral separation. These features are currently under investigation.



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P8

A fluorescent Zn(II)@hemicryptophane cage for heteroditopic recognition of phosphorylated choline

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Phosphorylated biomolecules play a central role in many biological processes and their fluorescent sensing may provide a unique tool to study their metabolism and other function.[1] Herein, we described a hemicryptophane combining a CTV unit, a Zn(II) metal center and fluorescent properties (figure 1).[2] This first fluorescent hemicryptophane has been developed as efficient fluorescent sensor for zwitterionic choline phosphate in competitive media. The heteroditopic character of the host towards the guest was evidenced since only the guest bearing both the ammonium and phosphate parts can give rise to the most significant fluorescent quenching and largest binding constant.[3] Moreover, it was found that the exchange between the free and complexed guest is slow on the NMR time scale at r.t. while fast at high temperature. NMR experiments also indicate the formation of an inclusion complex between the cage and guest, and a chiralization-like behavior of the achiral choline phosphate occurred. The binding mode have been highlighted by DFT calculations.

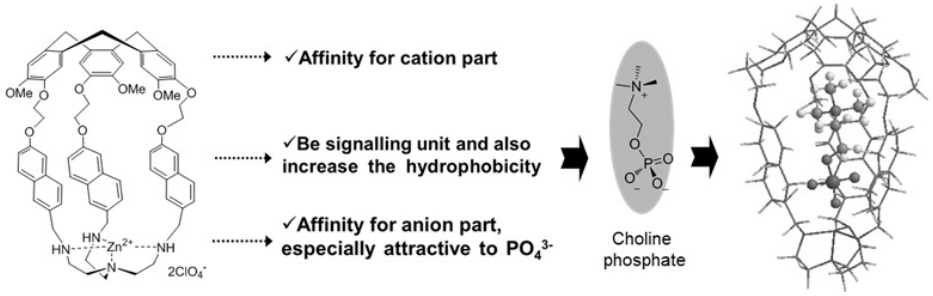

Figure 1 The structures of Zn(II)@hemicryptophane cage and choline phosphate, and the designing concept.

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P9

Switchable Molecular Tweezers: Luminescent or Magnetic

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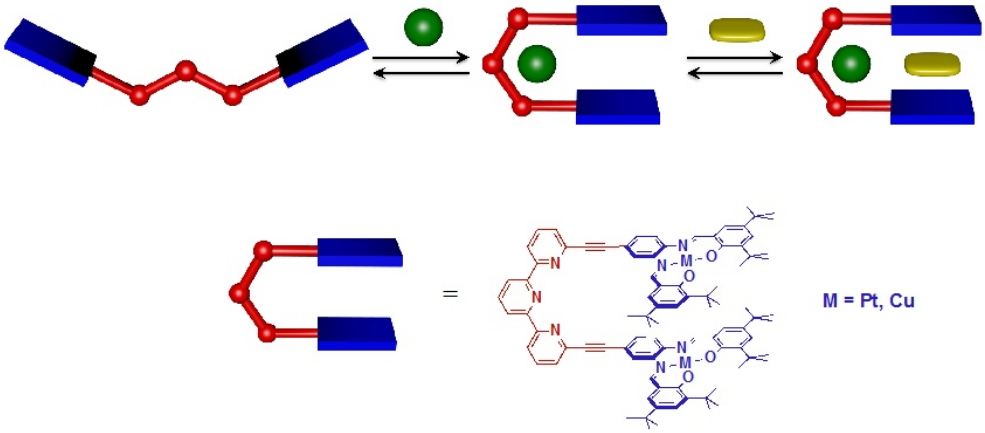
In the field of nanosciences, the control at the molecular level of physical or chemical properties represents an important challenge. Designing systems modular enough to permit reversible switching of optical or magnetic properties via a mechanical motion is an innovative approach. Supramolecular chemistry seems to be a key element to build such « on / off » systems based on molecular tweezers.[1] As a cooperative system, switchable molecular tweezers[2] offer the possibility of a double control of the physical properties due to the successive closure and guest intercalation.

We are interested in the design of molecular tweezers that are switchable by metal coordination.[3] Our system is based on a terpyridine ligand substituted in 6 and 6" positions by two arms bearing molecular recognition moieties. The terpyridine unit can switch upon metal coordination between a "W" shaped open form and a "U" shaped closed form bringing the two recognition units in an optimal geometry for binding substrates. Upon decoordination the tweezers will reopen, releasing the intercalated substrate. The recognitions units are based on salen complexes with magnetic or luminescent properties depending on the metallic center.

The design and synthesis of terpyridine(Pt-salen)2 based phosphorescent molecular tweezers will be presented as well as its reversible switching and the impact of intercalation on the luminescence properties.[4] A magnetic interaction switching by a mechanical motion in terpyridine(Cu-salen)2 molecular tweezers will also be presented.



Principle of a switchable molecular tweezers

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P10

Negative thermal expansion facilitated by weak host-guest interactions

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Reports of anomalous thermal expansion have become more frequent in recent years but are dominated by inorganic systems showing negative linear and volumetric thermal expansion. Typical examples include silicates and zirconium tungstenates that incorporate strong covalent bonds as well as MOF-5 and related IRMOFs constructed with metal-ligand coordination bonds.1 Organic compounds displaying these properties are still relatively rare.

Several mechanisms resulting in negative thermal expansion have been described. Arguably the most important of these have involved bridging atoms and rigid unit vibrational modes; magnetostriction; and electronic effects.2,3 Extremely large positive and negative thermal expansion for a dumbbell-shaped organic molecule was reported where the mechanism depended on a helical pattern of strong O-H•••O hydrogen bonds.4 For a multi-component organic hydrate recently reported as undergoing negative linear thermal expansion, an extensive network of ionic and hydrogen bonds is present.5

In the present study an 18-crown-6 solvate was investigated by variable temperature single-crystal X-ray diffraction. Exceptionally large positive thermal expansion in two axial directions and negative thermal expansion along the third was confirmed (figure 1). The mechanism of negative thermal expansion was determined and is unlike any previously described because it relies exclusively on weak electrostatic interactions. In fact, to our knowledge this compound displays the weakest directional intermolecular interactions of any organic material that undergoes negative thermal expansion.

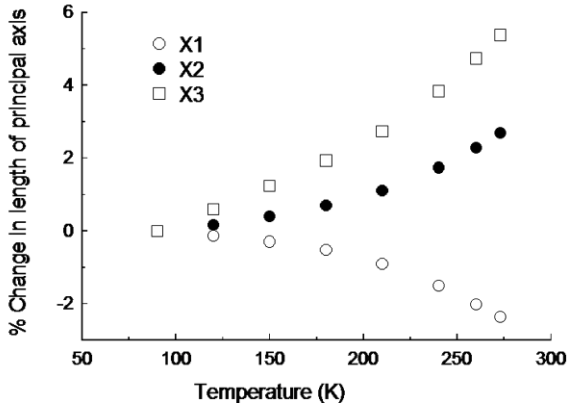

Figure 1: Percentage changes in principal axis lengths as a function of temperature.

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P11

Pre-assembled polymetallic precursors based on organophosphorus ligands for supramolecular assemblies

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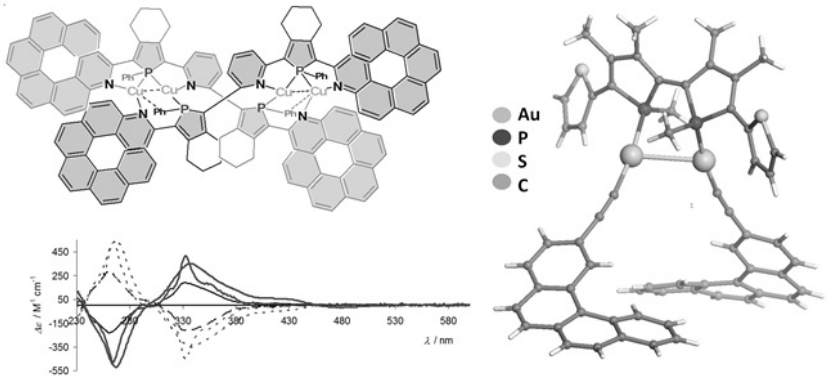
Our group develops synthetic strategies using coordination chemistry of organophosphorus derivatives to obtain functional supramolecular assemblies. We have described a family of air stable bimetallic complexes bearing the 2,5-bis(2-pyridyl)phosphole ligand as bridging phosphane ligand, a very rare coordination mode in the family of the phosphane ligands.[1] Among these, Cu(I) bimetallic complexes were used as versatile U-shape molecular clip in order to control the coordination-driven self-assembly of a variety of π-conjugated systems into π-stacked supramolecular metallocyclophanes.[2] These discrete metallacyclophanes self-organize into infinite π-stacked columns via intermolecular π-π interactions. This approach provides thus a rational strategy to control the solid state organization of π-conjugated systems and supplies solids in which an efficient charge transport across π-π stacked columns is expected.[3] This series of results highlights the interest of pre-assembled polymetallic precursors for coordination-driven self-assembly processes as well as of the use of multidentate ligands bearing bridging phosphane coordination modes. Recent progresses along these approaches will be presented.[4]



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P12

A Double Selection Process for Ion Transport Using Dynamic Covalent Chemistry

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Dynamic Covalent Chemistry (DCC) uses the reversibility of chemical reactions to build up thermodynamically controlled libraries.[1] For example, the reversibility of the reaction of amines with aldehydes or ketones allows the generation of dynamic covalent libraries (DCLs) of imines. By adding templates to these DCLs, members matching these templates can be amplified and the equilibria of the DCLs shift towards the matching products.[2]

An imine DCL is, for example, formed by the reaction of different oligoethyleneglycol diamines of varying lengths with a pyridinedicarbaldehyde. Upon addition of alkaline earth ions, different diimines can be amplified.[3]

Such a dynamic covalent imine library can be used directly for the selection of a carrier for transport (figure 1).[4,5]

First, template ions select hosts of matching size and amplify these. Matching macrocycles may possess different substituents Ri.

In a second selection process, the membrane selects the best carrier.[4,5] Results for differently substituted carriers will be presented.

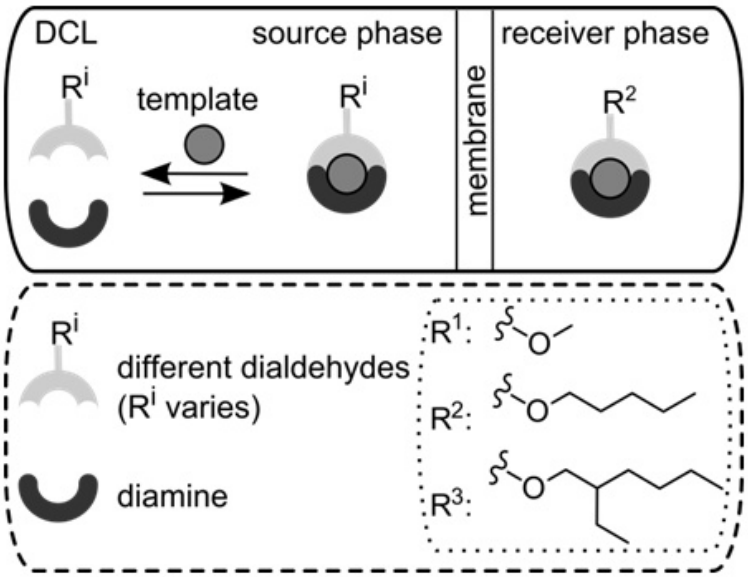

Figure 1: Ion transport across a supported liquid membrane (SLM) facilitated by a DCL. The template selects [1+1]-macrocycles and the membrane selects one substitution pattern (R2).

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P13

Formation of Polydiacetylenes From Higher Order Diiodopolyynes

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The formation of polydiacetylenes (PDAs) from triynes and longer polyynes has proven challenging due to the lower stability of these materials and the possibility of alternative regiochemistry for the polymerization. In this work, we have co-crystallized two diiodopolyynes, diiodohexatriyne and diiodooctatetrayne, separately with a Lewis basic host.1 Single crystal X-ray diffraction studies show that the halogen bonding interactions between the host and guest align the diiodopolyyne monomers with the proper parameters for 1,4-topochemical polymerization.2,3 Using Raman spectroscopy and solid-state 13C MAS-NMR we have demonstrated the formation of a highly ordered single PDA from the 1,4-polymerization of diiodohexatriyne, namely polyiodoethynyliododiacetylene (PIEDA) (Figure 1). Diiodooctatetrayne also forms ordered co-crystals with the host, but the resulting product is a disordered material. This work has demonstrated the first successful ordered 1,4-polymerization of a triyne using the host-guest method.

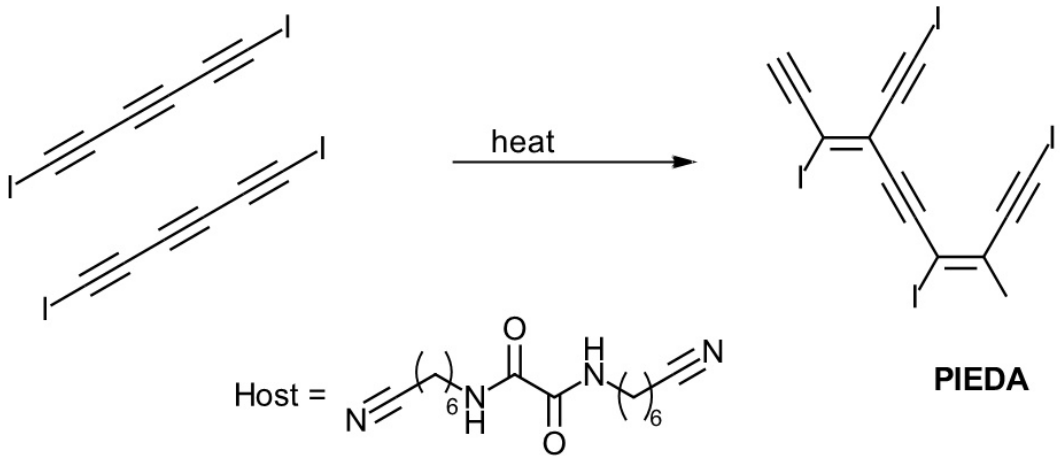

Figure 1. diiodohexatriyne in a monomer cocrystal (on left) will form polyiodoethynyliododiacetylene (PIEDA, right) when heated.

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P14 **Regioselective Spirocyclization of Biphenylacetylenes within a Hollow Cage**

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Biphenylacetylenes with a conjugated en–yne system undergo electrophilic cyclization to give phenanthrenes via 6-endo-dig cyclization. In this study, we found that octahedral hollow cage 1 encouraged selective 5-endo-dig cyclization of biphenylacetylene 2 by fixing its conformation to give spiro compounds 3.

Biphenylacetylene 2 was suspended in an aqueous solution of cage 1. After the mixture was stirred at 80 °C for 3 h, inclusion complex 1•2 was obtained in 70% yield (Figure 1a). To a solution of inclusion complex 1•2 was added N-bromosuccinimide and the resulting solution was further stirred at room temperature for 10 min. NMR measurements revealed that 5-endo-dig cyclization quantitatively proceeded to give spiro compound 3a. When N-iodosuccinimide was employed as an electrophile, 5-endo-dig cyclization proceeded selectively and spiro compound 3b was obtained in 75% NMR yield.

X-ray crystallographic analysis revealed π–π stacking between the substrate and panel ligands of the cage (Figure 1b). We consider that the conformational fixation of a reacting aromatic ring in the biphenyl moieties inhibits formation of a planar phenanthrene, leading to the regioselective spirocyclization.

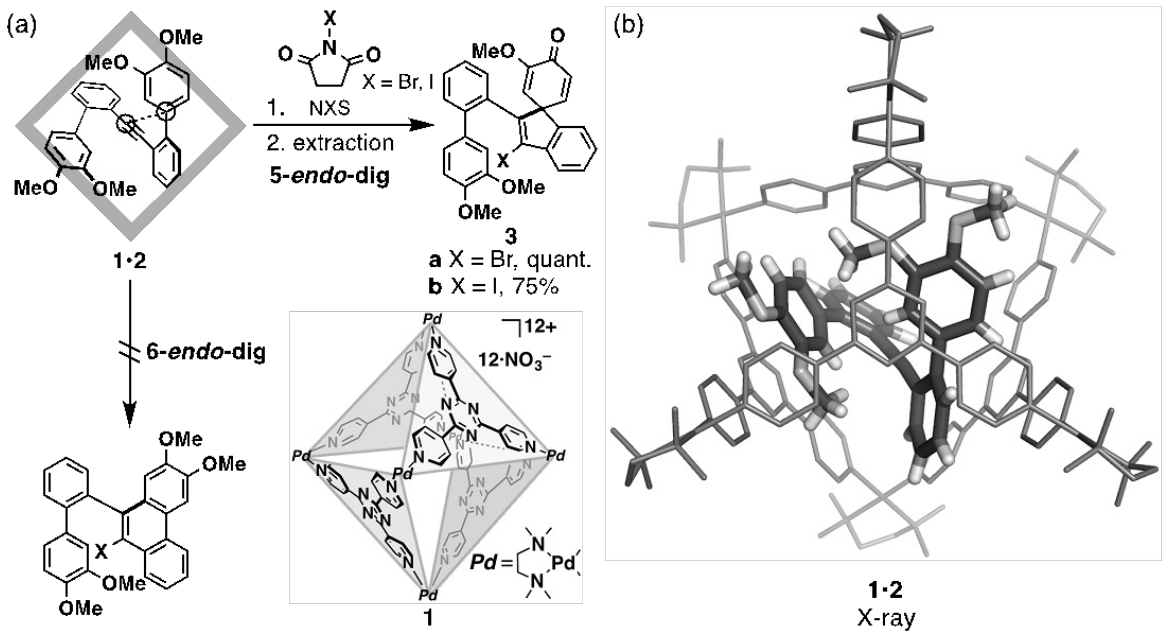

Figure 1. (a) 5-Endo-dig and 6-endo-dig cyclizations of biphenylacetylene 2. In cage 1, 5-endo-dig cyclization proceeds selectively. (b) X-ray structure of inclusion complex 1•2.

P15

Dynamic combinatorial libraries operated far from-equilibrium: toward dissipative molecular networks

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Dissipative, far-from-equilibrium systems are very common in the biological world but are still an exception in chemistry. The behavior of far-from-equilibrium systems is probably a lot richer than that of equilibrium systems but has yet to be explored. Therefore, we are trying to develop conditions where the components of dynamic combinatorial libraries (DCLs) based on disulfide chemistry are continuously cleaved and reformed via reduction and oxidation processes (Figure 1). These conditions can be named “recycling conditions” since the material is permanently part of a cycle a breakdown/reformation process. In order to allow these redox reactions to take place, oxidizing and reducing agents are continuously added to the library. This is the source of energy that drives the systems far from equilibrium and thus should enable us to observe new states that cannot be reached in absence of this continuous flow of energy.

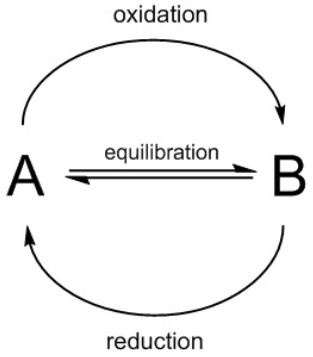

Figure 1. Schematic representation of the processes taking place in the DCL: oxidation and reduction reaction are depicted as irreversible processes and equilibration via exchange is represented by an equilibrium arrow.

Our first experiments clearly demonstrated that a detailed understanding of the kinetics of all steps in the system processes is essential to achieve the desired conditions. In the conditions we initially used (neutral pH, ≈ 80 % oxidation...), reorganization (equilibration via exchange reactions) was found to be too fast to be influenced by the imposed redox reactions. Thus, we have turned to an investigation of the separate redox and exchange rates under a broad range of conditions with the intent, aided by computational modeling, that once conditions are found where oxidation and reduction are faster than exchange processes we will apply them first to DCLs based on building blocks developed in our laboratory, investigating template effect. Then, these “far-from-equilibrium” conditions will be applied to self-replicators emerging from DCLs, where the recycling conditions should allow us to observe Darwinian evolution in fully synthetic self-replicating systems.

P16 **Molecular tectonics based nanopatterning of interfaces with 2D metal-organic frameworks (MOFs).**

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The functionalization of surface by molecular assemblies with sub nanometer precision and long range order is one of the current challenges in nanoscience [1]. The generation of molecular networks on surfaces, i.e. periodic architectures displaying translational symmetry, may be achieved using the molecular tectonic approach based on tecton-tecton and tecton-surface specific interactions. Indeed, molecular tectonic deals with the design and construction of infinite periodic architectures in the solid state through selfassembly processes between programmed building blocks named tectons. Due to their unique opto-electronic properties, the surface patterning using porphyrins based tectons could generate material displaying interesting applications such as in solar cells [2] or in catalysis [3].

Herein, we present the formation of 2D coordination networks generated at the solid-liquid interface on graphite surface (HOPG). The formation of periodic arrangements was monitored by STM. The architectures resulted from the interconnection of an acentric porphyrin tecton (P) bearing two different pyridyl units and the neutral complex CoCl2 as four connecting node. Interestingly, among the different possibilities, the 2D network with the highest symmetry is formed under conditions used (figure 1) [4].

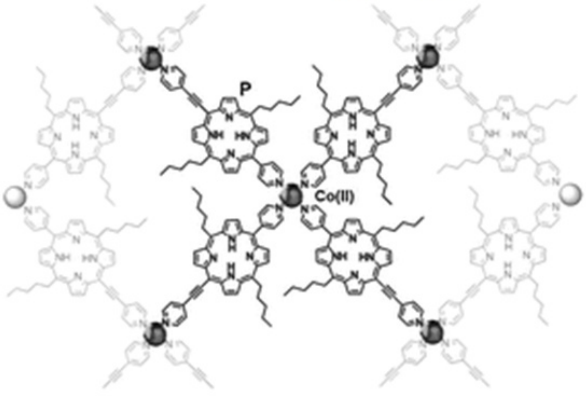

Figure 1: Representation of the 2D network formed upon combining the porphyrin P and CoCl2

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P17

Azadipyrrin based heterometallic coordination networks

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Molecular tectonics, an approach at the interface of Supramolecular/coordination and solid state chemistry, deals with the design and description of molecular networks in the crystalline phase.[1] Over the past two decades, coordination networks and metal organic frameworks (MOFs) have attracted considerable interest owing to their possible applications.[2] These architectures are based on the interconnection of metal cations or complexes and organic tectons. Regarding the latter, dipyrrin derivatives of the bis-pyrrolic type,[3] have been used for the formation of both homo- and heterometallic coordination networks.[4] Unexpectedly, their analogues bearing a nitrogen atom in the position 5 named azadipyrrin have not been explored for the formation of periodic architectures. This is surprising since these compounds, monoanionic chelates under basic conditions, can be readily synthesized and functionalized. In particular, reaction with boron leads to azaborondipyrromethene (azaBODIPY) which have been studied for their photophysical properties.[5] The use of such luminescent molecules as metalloligands or metallatectons may thus afford novel emissive heterometallic coordination networks (Figure 1). Along these lines, we shall present here our recent results on a novel azadipyrrin based tecton.

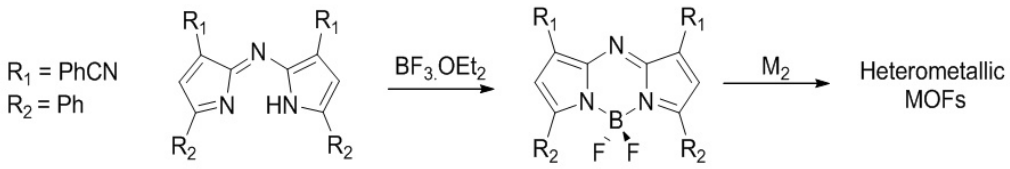

Figure 1 Step by step synthesis of azadipyrrin based heterometallic coordination networks.

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P18

Unveiling the nature of supramolecular crown ether-C60 interactions

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Construction of artificial photoactive devices capable of mimicking photosynthesis by transforming light into chemical potential is one of the most sought objectives in the quest for new sources of energy.[1] For this, chemists have developed a wide variety of covalent and supramolecular structures based on donor-acceptor systems where photon energy is used to produce a photoinduced electron-transfer from the donor to the acceptor moiety.[2]

As a result, in 2010 our group developed a supramolecular exTTF-B18C6 ether receptor for fullerenes which showed an extraordinary affinity (Ka 5.01 × 106 M-1) towards [60]fullerene.[3] This was an outstanding result as previous attempts to complex fullerenes by only one unit of exTTF were unsuccessful. Thus, the presence of crown ethers as recognition patterns seemed to be of paramount importance.

In this work, we have further studied this unexpected result and exploited the potentiality of crown ethers as recognition motifs for fullerenes. Therefore, we have synthesized a new series of exTTF–(crown ether)2 platforms where both the impact of size modification and the introduction of heteroatoms (i.e. nitrogen) towards the affinity to C60 have been studied by spectroscopic and computational methods (figure 1).

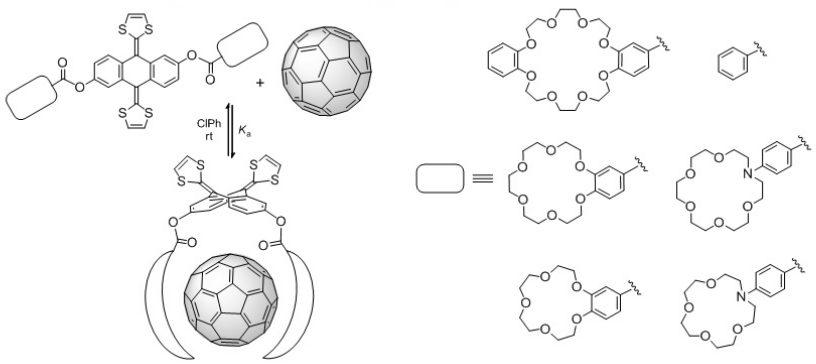

Figure 1. Complexes obtained from exTTF based tweezers

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P19

Three-dimensional Au(I) arrays on a tray-shaped Au3 scaffold

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Precise synthesis of metal ion clusters has attracted increasing interest for understanding of those properties depending on the species, number, and array of component metal ions. Here, we demonstrate that tray-shaped Au(I)3Pd(II)3 complex serves as a molecular scaffold for discrete stacks of planar trinuclear Au(I)3 complexes to produce three-dimensional [3 (n] Au(I) ion arrays. The stack number of Au(I)3 planes (n) is systematically controlled (n = 2–4) by solvent conditions and addition of Ag(I) ions.

Tray-shaped Au(I)3Pd(II)3 complex 1 self-assembled from a cyclic trinuclear Au(I)3 complex functionalized with six 3-pyridyl groups and three equivalents of Pd(II) hinges (Figure 1a). In the shallow concave cavity provided by the peripheral pyridyl groups, guest Au(I)3 complex 2 stacked and formed Au(I) clusters. In a H2O/CH3CN (7:3) mixed solvent, tray 1 and guest 2 aggregated in a 1:1 ratio to form Au3–Au3 metal ion cluster 1•2 in 93% yield (Scheme i in Figure 1a). In water, two molecules of tray 1 sandwiched one guest 2 to give Au3–Au3–Au3 metal ion cluster 1•2•1 quantitatively (Scheme ii). Moreover, addition of Ag(I) ions in the system gave Au3–Au3–Ag–Au3–Au3 metal ion cluster 1•2•Ag+•2•1 (Scheme iii). Solution NMR spectroscopy and single crystal X-ray analysis revealed that two trays 1 sandwiched the dimer of guest 2 to form quadruple Au(I)3 stack and that one Ag(I) ion located at the center of the ion cluster (Figure 1b). The short intermolecular Au···Au and Au···Ag distances indicated the existence of Au(I)···Au(I) and Au(I)···Ag(I) interactions, respectively. In particular, the Ag(I) ion effectively worked as a glue to connect two Au3–Au3 double stacks 1•2 in a face-to-face fashion.

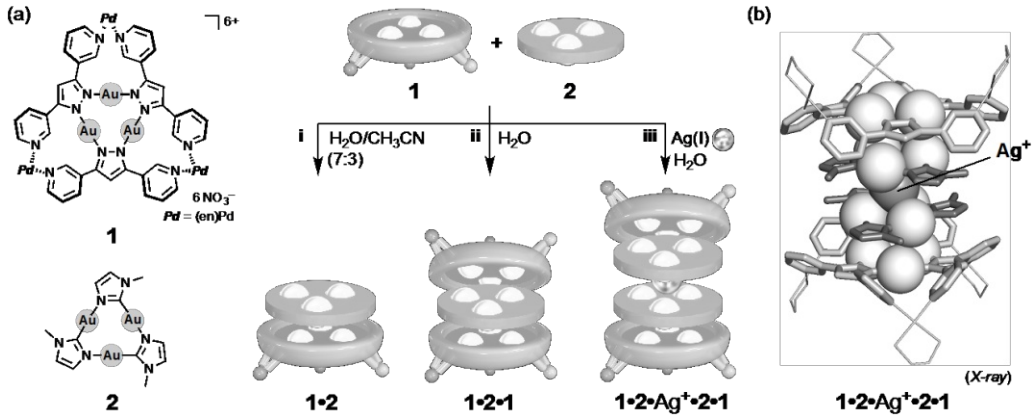

Figure 1. (a) Schematic representation of the formation of double, triple, and quadruple Au(I)3 stacks. Tray-shaped Au(I)3Pd(II)3 host 1 accommodated guest Au(I)3 complex 2 to form a variety of Au(I) ion clusters depending on the conditions. (b) X-ray crystal structure of Au3–Au3–Ag–Au3–Au3 metal ion cluster.

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P20 **Linear and Cyclic Peptide based Boronic Acid functionalized Carbohydrate Receptors**

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Carbohydrate recognition plays an important role in various biological processes like cell-cell recognition, inflammation and infections of cells by viruses and bacteria. Embedded in cell membranes in form of glycoproteins and glycolipids, carbohydrates take part in protein-carbohydrate interactions at the cell surface.[1] To understand these processes the development of synthetic carbohydrate receptors is crucial.

Since a long time it is known that phenylboronic acids have a high affinity to bind diols.[2] This property makes phenylboronic acids an interesting structural element for the field of carbohydrate recognition. In the literature both cyclic[3] and linear[4] peptide based phenylboronic acid functionalized carbohydrate receptors are known. We report a peptide based phenylboronic acid functionalized receptor that can work as both linear and cyclic receptor due to dimerization of the thiol functions (figure 1). Herein, we show the synthesis and the determination of the binding constants from various carbohydrates to these receptors via ITC measurements and fluorescence titration experiments[5].

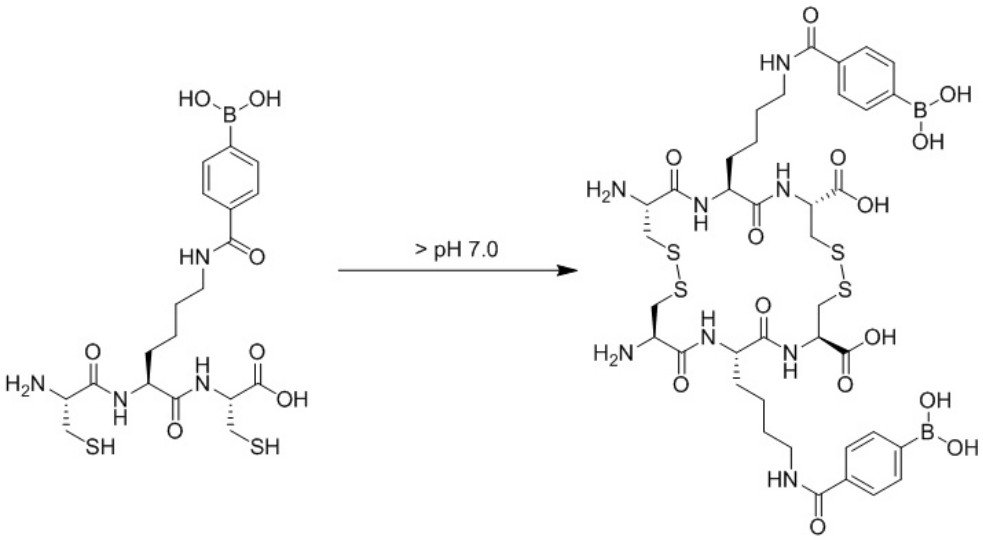

Figure 1: Structure of the linear and cyclic peptide based carbohydrate receptor.

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P21

Functionalized Cyclodextrin Polyrotaxanes for Bimodal Imaging

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The understanding of biological mechanisms and the development of powerful tools for diagnostic should make the most out of all recent progress that have been achieved in the in vivo imaging area.[1] Actually, the use of multimodal imaging can take advantage of complementary properties such as resolution, sensitivity, penetration, targeting or compatibility.

In our project, a cyclodextrin polyrotaxane was chosen to be the backbone of a modular multimodal platform for in vivo imaging.[2] This supramolecular structure allows flexibility and modularity for probe combinations and potential biocompatibility provided by the cyclodextrin units. In a first approach, fluorescence imaging and magnetic resonance imaging were combined for the high sensitivity of the former and the good spatial resolution of the later.[3] In a building blocks strategy, molecular probes were first connected to an α-cyclodextrin and then threaded onto a polyammonium axle to form bimodal polyrotaxanes.

The synthesis of functionalized α-cyclodextrins with fluorescent probes such as BODIPY or cyanine-5 and with a Gd complex as MRI contrast agent will be presented as well as their self-assembly and characterization of the mixed polyrotaxane.[4]

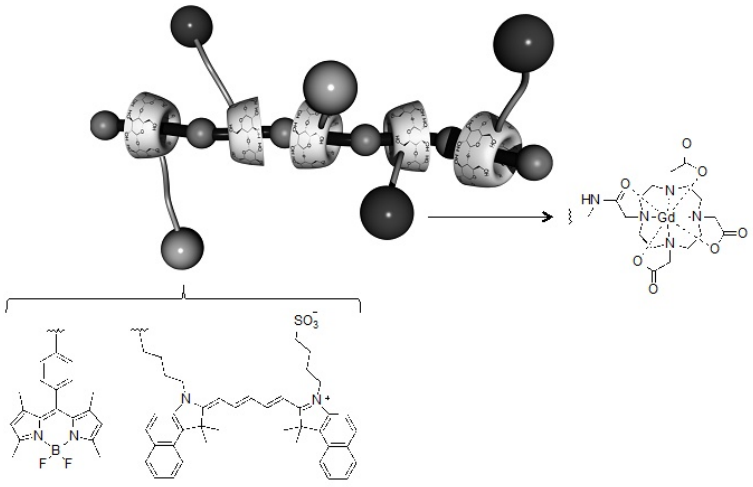

Figure: Polyrotaxane with cyclodextrins functionalized by a fluorescent tag (left) and contrast agent for MRI (right)

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P22 **Self-assembled architectures with segregated donor and acceptor units of a new monopyrrolo-TTF-PTM radical**

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Organic molecules which contain electron donor (D) and electron acceptor (A) units linked by π-conjugated bridging groups (D-π-A dyads) are worthy of attention for the investigation of intramolecular electron transfer (IET) processes and in some cases for their associated bistability phenomena [1]. Recently, we have reported the D-A system based on a tetrathiafulvalene (TTF) electron π-donor connected to the polychlorotriphenylmethyl (PTM) radical electron acceptor by a vinylene bridge [2]. This radical dyad present bistability in solution existing in the monomeric neutral or in the dimeric charge separated state and exhibit different optical, magnetic and electronic properties in each one of the state. Such bistability can be switched playing with external stimuli such as the concentration, polarity of the solvent or temperature [2-4]. Regarding the potential applications as electronic and optoelectronic devices, there is a high interest in obtaining TTF-based D-A systems that exhibit molecular packings with a complete segregation of the donor and acceptor fragments forming homostacks of the TTF subunits, since this is an important prerequisite for attaining electronic conductivities. Herein we report a new electron donor-acceptor dyad 1 based on a PTM radical subunit linked to a TTF unit through a π-conjugated N-phenyl-pyrrole-vinylene bridge that has been synthesized and fully characterized. The intramolecular electron transfer (IET) process and magnetic properties of the radical dyad have been evaluated by cyclic voltammetry as well as UV-Vis and ESR spectroscopies both in solution and in solid state. The self-assembling ability of the radical dyad has been investigated by X-ray analysis showing supramolecular architectures with segregated donor and acceptor units where the TTF subunits are stacked forming 1-D chains. Analysis of the bond lengths obtained by X-ray diffraction reveals certain degree of intramolecular charge transfer in the solid state upon decreasing the temperature.

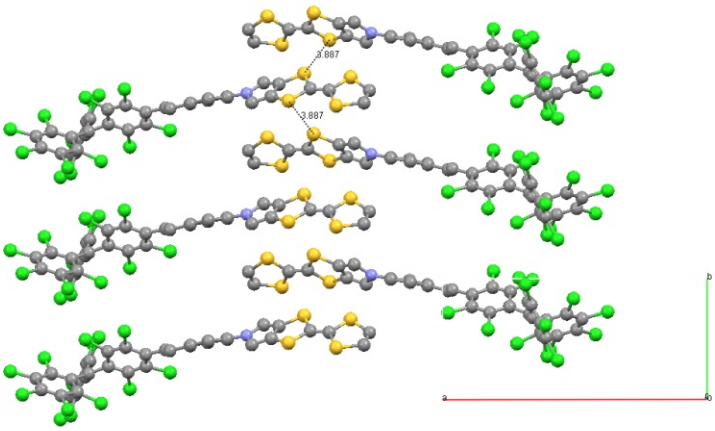

Figure 1. Molecular packing of 1 in the ab plane.

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P23 **X-ray Crystallographic Analysis of Organometallic Compounds Using Crystalline Sponge Method**

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Organometallic chemistry greatly owes its progress to x-ray crystallography because compounds with carbon-metal bonds are in most cases hardly characterized only by spectroscopic methods such as NMR and IR. However, single crystal preparation of organometallic compounds, inevitable for their x-ray analysis, is not always an easy process because of their air- and moisture-sensitive natures frequently encountered. Here, we report the structure analysis of organometallic compounds by recently developed crystalline sponge method1,2 that does not require the crystallization of target samples. By showing the crystal structures of some organometallic compounds including non-crystalline ones, we expand the scope of the method and demonstrate that the crystalline sponge method will be a great help for organometallic studies.

In this work, porous coordination network [(ZnI2)3(tpt)2]n (1; tpt = tri(4-pyridyl)-1,3,5-triazine) were used as a host framework. According to optimized conditions for analysis of organic compounds, we conducted encapsulation of ferrocene molecules into the host complexes. 5 µg of ferrocene (2) dissolved in 50 µL cyclohexane were added to one crystal of 1 (solvent = cyclohexane; 120 × 60 × 50 µm3) placed in a microvial. The solvent was slowly evaporated at 50 ˚C over 2 d and the resulting crystal was subjected to single-crystal X-ray analysis. Although the crystal structure thus obtained showed relatively large residual electron densities assignable to iron atoms, whole structure of ferrocene was not refined because of low occupancy (ca. 53%). When 10 µg of ferrocene was used under the milder conditions (r.t. over 4 d), the structure of ferrocene was clearly determined with high occupancy (ca. 93%)(figure 1(a)). With these optimized conditions, we also analyzed various organometallic compounds. Mn-carbonyl compound 3 and Ir(COD) complex 4 were unambiguously determined in a similar fashion without ligand exchange. To our delight, even reactive tin-hydride complex could be analyzed with out procedure without any decomposition or side reaction(figure 1(b)).

These results demonstrate that our crystalline sponge method is useful for the structural analysis of organometallic compounds.

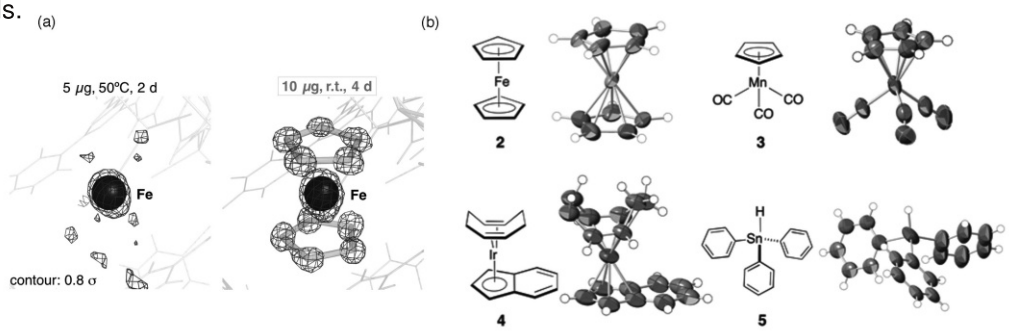

Figure 1. (a) Comparison of the observed electron density maps (Fo) around the ferrocene guest: (left) under the previously optimized conditions for organic molecules, (right) newly optimized conditions. (b) ORTEP drawing of 2, 3, 4 and 5 with 30% probability ellipsoids, which were analyzed under newly optimized conditions.

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P24 **Towards Speciation in Self-Replicating Systems Containing Mutated Building Blocks**

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Self-replicating systems play an important role in studies concerning the origin of life.1 In our group, self-replicating molecules based on peptidic building blocks are widely studied in which the key idea is building up dynamic combinatorial libraries of macrocyclic molecules of different ring sizes that can exchange building blocks through reversible disulfide exchange. Preliminary results suggest that multiple replicators differing in their ring sizes compete for the same building block which can result in the formation of large macrocycles up to 8mer.2

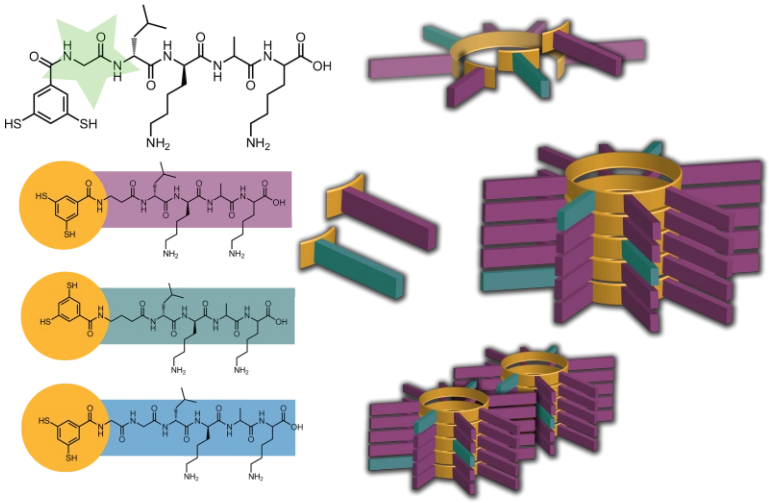

Figure 1. Cartoon representation of mutated building blocks (left) and self-replication. In Dynamic combinatorial libraries, these building blocks form macrocycles with different ring sizes in which the system is under thermodynamic equilibrium. In such a system, if one of the macrocycles can catalyse the production more copies of itself, they form fibres that elongates to an extent. Under mechanical agitation these fibres break and the produce more fibre ends. The more the fibre ends in the system, the more efficient the replication occurs.

In this study, the aim is to change the composition and/or the size of the replicating macrocycles by allowing it to mutate by the incorporation of different building blocks (figure 1). Building blocks contain a structurally different spacer between the exchange unit and the peptide sequence. Preliminary results suggest that, building blocks containing Gly-Gly and gamma aminobutyric acid can transform homogeneous octamers into heterogeneous trimer and tetramers. On the other hand, when the spacer is beta alanine, the system behaves unexpectedly: this building block leads to the formation of the unprecedentedly large macrocycle.

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P25

LIGHT-DRIVEN HYDROGEN-BONDED [2]ROTAXANE FORMATION

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Mechanically-interlocked molecule synthesis typically relies on preorganization or templating using self assembly, for example harnessing noncovalent interactions between a molecular guest thread and a macrocyclic host [1], before covalent capture of the dynamic interpenetrating ensemble. Hydrogen bonds, with their inherent directionality, allow the binding of neutral molecules using multiple hydrogen bonds. One of the most successful receptors for complexation of neutral molecules is Hamilton's barbiturate receptor.[2] We recently harnessed this receptor:barbiturate motif (see Figure 1a) for pseudorotaxane formation using a macrocylic version of the receptor.[3] Subsequently, [2]rotaxane formation was realized via a stoppering reaction using a copper(I)-catalyzed alkyne-azide 1,3-cycloaddition click reaction.[4] Here we report rotaxane formation via photoclipping of a Hamilton-like receptor bearing photodimerizable anthracene groups onto a molecular thread as a strategy to give organic bead-on-thread structures, see Figure 1b.[5]

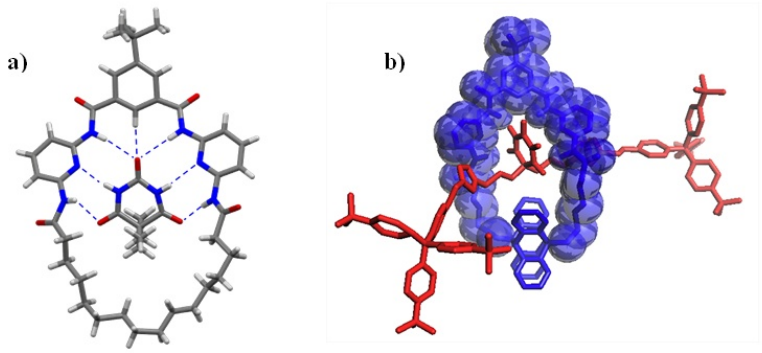

Figure 1. a) X-ray structure of related molecular host-guest complex, b), MM3 modeling structure of the [2]rotaxane obtained via photoclipping.

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P26

Self-Assembly of M30L60 Icosidodecahedron

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Construction of a series of giant MnL2n coordination polyhedra by self-assembly is a strong demonstration that coordination self-assembly goes to protein assembly being able to precisely control chemical structures on the nano-scale. From geometrical constraints, only n = 6, 12, 24, 30, and 60 were allowed for the MnL2n regular or semi-regular polyhedral structures and to date those with n = 6, 12, and 24 have been synthesized (Fig. 1).1 Here we report the self-assembly of a M30L60 ninety-component complex whose symmetry is described as icosidodecahedron with thirty vertices and sixty edges.

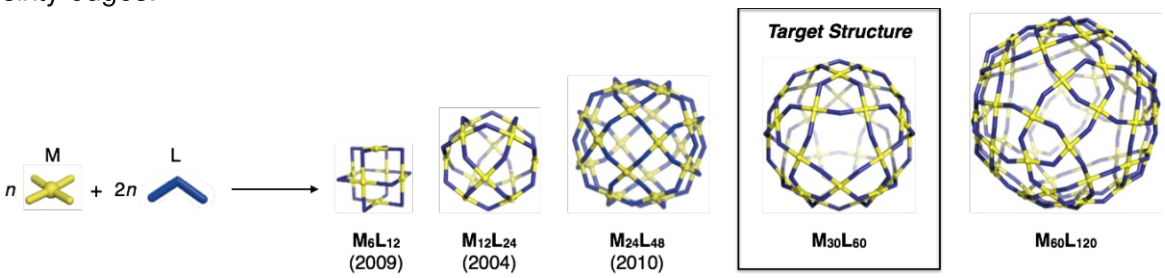

Figure 1 Schematic image for self-assembly of MnL2n polyhedra

We newly synthesized bidentate ligand 1 and examined complexation of 1 and Pd(BF4)2(CH3CN)4 in DMF. 1H and 1H DOSY NMR spectra indicated quantitative formation of a large complex with (Fig. 2). Single crystals of complex 2, suitable for synchrotron X-ray crystallography, were obtained by very slow vapor diffusion of AcOEt into a solution of 2. The crystal structure of 2 revealed ninety-component self-assembly and the largest well-defined coordination polyhedron reported so far, with the diameter of ~8.2 nm (Fig. 3).

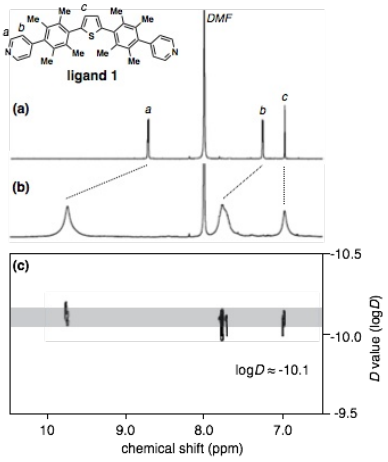

Fig. 2 1H NMR spectra of (a) ligand 1 and (b) complex 2. (c) DOSY spectrum of complex 2 (500 MHz, 300 K, DMF-d7)

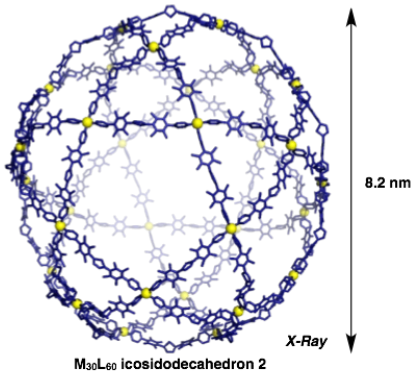

Fig. 3 Crystal structure of M30L60 icosidodecahedron 2

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P27 **Molecular tectonics: fluorinated porphyrin based coordination networks**

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Since the introduction of a fluorine atom to the 9α position of cortisol in 1954,1 fluorine atom is found in ca 15-20% of new chemicals licensed each year in pharmaceutical products and up to 30% in agrochemicals.2 As the role played by fluorine atom in everyday life is constantly increasing, it is worth investigating its impact on physical, chemical, biological and structural properties in functional materials.3

Porphyrin derivatives, biologically relevant macrocycles, have been intensely studied due to their interesting features such as robustness, thermal stability and their propensity to bind a variety of metal cations by their macrocyclic tetraaza core or by appended coordinating sites. 4 One may combine the above mentioned characteristics of the porphyrin backbone and the peculiar behavior of fluorine atom by connecting to the backbone fluorine enriched fragments. Furthermore, following principles developed in molecular tectonics,5 such molecular entities bearing peripheral coordinating sites may behave as tectons (building blocks) for the generation of fluorinated coordination networks of interest for the separation of fluorinated compounds through fluorine-fluorine interactions.

Herein we present the synthesis of novel porphyrin based tectons bearing two fluorinated alkyl chains and two pyridyl coordinating sites at opposite meso positions. Furthermore, we report on the structural features of coordination networks of different dimensionality obtained upon their combinations with metal cations or metal complexes (figure 1).

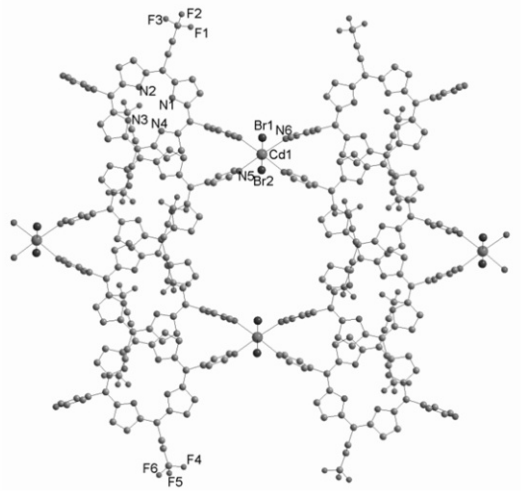

Figure1. An example of a 2D fluorinated network obtained with Cd2+ metal cation.

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P28 **A Self-Assembled M3nLn Coordination Capsule with Large Structural Change for Guest Encapsulation**

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Constructing huge artificial capsules has drawn great attention because the highly isolated nanocavities can recognize large guest molecules. Hitherto, many molecular capsules have been created with various huge hollow structures; however, providing molecular recognition abilities has still been a challenging. In this work, we designed a self-assembled coordination capsule for the encapsulation of large guest molecules by its dynamic structural change property.

Previously, we reported a M18L6 hexahedral capsular framework but it displayed poor guest encapsulation behavior.1 To enhance the molecular recognition abilities, here we designed a new electron-deficient ligand, 2,4,6-tris(3,5-pyrimidyl)-pyrimidine (L). When M and L were mixed in 3:1 molar ratio in water for 24 h at 70 oC, a highly symmetrical M18L6 hexahedral capsule was quantitatively formed as confirmed by NMR and crystallographic analysis. However, when acenaphthylene was suspended to this solution, the capsular structure was dramatically changed. In 1H-NMR spectrum, sharp aromatic signals of M18L6 capsule were completely changed into broad signals. Single crystal X-ray analysis clearly revealed the formation of M24L8 capsule encapsulating four molecules of acenaphthylene (figure 1).

Moreover, the typical host molecule, calix[4]arene, could also be encapsulated within the cavity of M24L8 capsule, as confirmed by NMR measurements and crystallographic analysis. These encapsulation abilities were enabled by not only the ligand interactive property but also dynamic nature of the coordination capsule. The change of inner cavity volume from M18L6 to M24L8 capsules was estimated as 304 to 923 Å3 (VOIDOO, probe 3.36 Å). Thus, we successfully created a huge molecular capsule with strong guest binding ability by intrinsic dynamic nature.

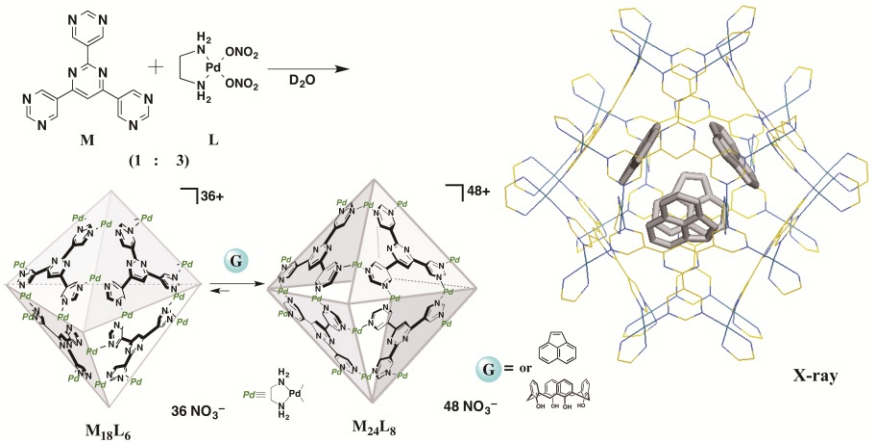

Figure 1 Scheme of M3nLn capsular formation and crystal structure of M24L8 capsule (guest: acenaphthylene).

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P29 **Synthesis of Chiral Iridium complexes for the formation of Coordination networks**

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Chiral and luminescent metal-organic porous materials have drawn more and more attention because of their potential applications in chiral separation, gas storage, and asymmetric catalysis [1-3]. Six coordinated Iridium complexes, well-known for their efficient emission properties, may be chiral with either Δ or Λ configurations depending on ligand used. We aim at the design and synthesis of new enantiopure iridium complexes (figure 1) [4] and their use as tectons for the generation of chiral coordination networks using the molecular tectonics strategy [5]. In order to transform enantiopure iridium complexes into coordinating tectons, they have been functionalised with peripheral divergently oriented pyridyl moieties acting as coordinating sites towards metal cations for the formation of molecular networks through selfassembly processes. In order to perform selective incorporation of fluorinated guest molecules within the pores of the network, the chiral Ir based tectons may be decorated with fluorine atoms.

In this poster, the synthesis of both racemic and enantiopure Iridium complexes as well as their use as metallatectons for the formation of coordination networks is described.

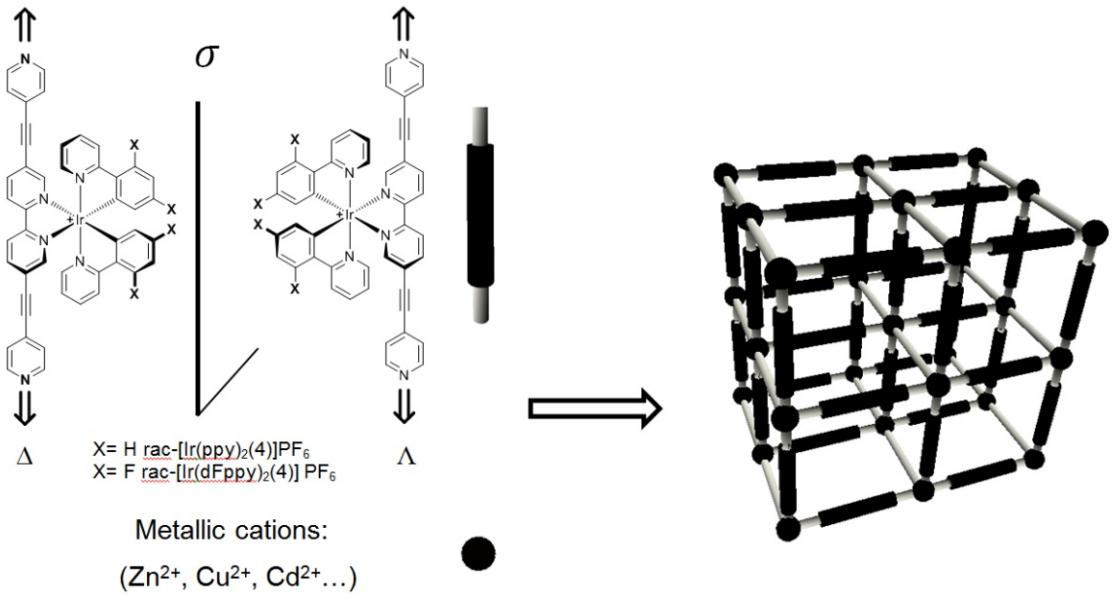

Figure 1: structures of Ir based chiral tectons and schematic representation of a possible 3D porous network.

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