The Satellite Symposium on Soft Crystals

UNIVERSITÉ DE STRASBOURG

The 7th International Mini-symposium on Advanced Coordination Chemistry 5 July, 2018, 10:00-18:00



Salle Mauve, Faculty of Chemistry University of Strasbourg, France

Organizers: Miki Hasegawa • Mir Wais Hosseini • Hitoshi Goto

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Under the auspices of MEXT KAKENHI, Innovative area "Soft Crystals"

10h05-10h35

Crystal Engineering for Enantioseparation - Diastereomeric Salt and Conglomerate Salt Formations -Kazuhiko Saigo

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The enantioseparations by diastereomeric salt formation and by conglomerate salt formation are fascinating methods for obtaining enantiopure compounds, as well as chirality pool method, asymmetric synthesis, and chiral chromatography. However, there were no study on factors/mechanism, which lead to satisfactory enantioseparations, when we started our research in this field; most of papers reported only successful results. Under such circumstances, we considered that necessary and important would be systematic studies on the enentioseparations using a structure-related series of components for diastereomeric salt conglomerate salt formations.

Diastereomeric Salt formation

We carried out systematic study on the enantioseparation (the diastereomeric salt formation) of racemic 1-phenylethylamine derivatives with enantiopure mandelic acid (resolving agent) and found that there is high correlation between success or failure of the enentioseparation and the position of a substituent on the phenyl group of 1-phenylethylamine derivatives. On the basis of the results, we proposed "principle of relative molecular length" for success enantioseparation. In the next stage, we applied 2-(2-naphthyl)propanoic acid and 2-(6-methoxy-2-naphthyl)propanoic

acid for the enantioseparation of racemic amines to find another factor, "principle of aromatic rings" we called.

Conglomerate Salt Formation

On the basis of the successful enantioseparation (the conglomerate salt formation) of the salt of racemic 1-phenylethylamine with achiral cinnamic acid (derivatizing agent), we tried to elucidate the role of the derivatizing agent in conglomerate salt formation. As a result, we found that "principles of relative molecular length and aromatic rings" are applicable for the explanation of the success.

Bridge Between Enantioseparations by Diastereomeric Salt and Conglomerate Salt Formations

Thus, the success in enantioseparations by the diastereomeric salt and conglomerate salt formations are governed by common principles. The thorough examination of possible crystal modifications of diastereomeric salt and conglomerate salt crystals led us to find a new bridge between diastereomeric salt and conglomerate salt formations.





SOFT CRYSTALS



10h35-11h05

Approach to Soft Crystals: toward investigation of their phase transition mechanisms Hitoshi Goto

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"Soft crystals" are a brand-new class of particular molecular materials that are "hard" crystal structures but easily change to another form by specific low energy stimulation at room temperature. There are still many mysteries on their crystal formation and phase transition phenomenon, but discovery and creation of innovative material functions is strongly expected. In our study on this new project, some new computational technologies are developed to build the theory for the formation and transition mechanism of the novel crystals, and here we will introduce a part of them [1,2]; (1) construction of a crystal force field that can precisely and promptly evaluate their molecular crystal structure formed by organic compounds and organometallic complexes, (2) developments of an efficient crystal polymorphic structure search method and (3) their phase transition dynamics simulation. Our first targets are two soft crystals: (a) phenyl-(phenylisocyanide) gold complex [3] and (b) terephthalamide [4] as shown in Figure. In this symposium, we will present tentative results of phase transition dynamics simulations based on the crystal vibrations (phonon modes) and try to give some theoretical interpretations to their phase transition phenomena.

This work is supported by JSPS KAKENHI Grant Number JP17H06373.



Figure (right) Optimized crystal structure of phenyl isocyanide gold complex form IIy and the lattice vibration vector (phonon mode) corresponding to 4th lower frequency.

- 1. Goto, H.; Obata, S.; Nakayama N.; Ohta, K. CONFLEX 8; Conflex Corporation, Tokyo, Japan, 2017.
- Reilly, A. M.; et. al. Acta Crystallographica Section B 2016, 72 (4), 439-459.
- 3. H. Ito, *et. al.*, Nat. Commun., 2013, 4, 2009; T. Seki, *et. al.*, J. Am. Chem. Soc., 2016, 138, 6252.
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11h30-12h00

Luminescent Lanthanide Complexes with the Helicate Molecular Structure Toward to the Soft Crystals Miki Hasegawa

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Owing to their chirality and optical properties, helical luminescent architectures have lately attracted considerable interest in material science. Based on rare earths coordination cdompounds, the synthesis of strategic helicate molecules displaying luminescence or magnetic properties has been reported [1]. We have designed helical mononuclear f-complexes based on hexadentate organic ligands and investigated their photophysical stability in solution. Figure shows the solid-state structures obtained by X-ray diffraction on single crystal X-ray structure of a series of f-coordinating helicates based on an organic ligand consisting of two bipyridine moiety bridged with ethylendiamine [2]. The energy donor level of the ligand efficiently acts for their ff transitions via intramolecular energy transfer in organic solutions and in ionic liquids[3]. The introduction of carboxyl groups on the ligand backbone, renders these complexes soluble in water. Interestingly, in aqueous media, the f-complexes display stable luminesce in a wide pH range, 2.6-11.4 [4]. Recently, the addition of acyl group with alkyl chains into the mother complex results in the unexpected coordination mode [5]. The Eu ion dissociates five chelate rings dissociate in the complex, instead of the coordination with oxygen atoms belonging acyl groups.

 $Pr \qquad Nd \qquad Sm \qquad Eu \qquad Gd \qquad Tb \qquad Dy \qquad Ho \qquad Tm$

Figure (top) Observed structure of mother molecule, EuL, and (b) sideviews of a series of LnL.

- 1. J.C.G. Bünzli, et al., Coord. Chem. Rev., 2010, 254, 2623.
- 2. M. Hasegawa, et al. New J. Chem., 2014, 38, 1225.
- 3. Yuki Hasegawa, A. Ishii, M. Hasegawa, et al., Molecules, 2018, 23, 55
- 4. S. Ogata, M Hasegawa, et al., New J. Chem., 2017, 41, 6385.
- 5. S. Ogata, M. Hasegawa, et al., *Dalton Trans.* 2018, 47, 7235.





SOFT CRYSTALS

14h00-14h30 CHIRALITY IN MOLECULAR TECTONICS

Mir Wais Hosseini

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Chirality plays a fundamental role in biology. In synthetic chemistry, considerable efforts have been devoted to control the chirality. The design and construction of chiral extended architectures is of prime importance for chiral separation and chiral catalysis. More specifically, the formation of enantiomerically pure crystals is rather challenging. Applying the concepts developed in molecular tectonics^[1] based on combinations of informed construction units (tectons) and connecting units, the design of enantiomerically pure extended architectures may be achieved using either enantiomerically pure organic tectons or enantiomerically pure metal complexes as nodes of the network.



A variety of chiral crystals will be presented.^[2]

a) M. Simard, D. Su, J. D. Wuest, (1991), J. Am. Chem. Soc., 1993, 113, 4696;
 b) S. Mann, Nature, 1993, 365, 499; c) M. W. Hosseini, Acc. Chem. Res., 2005, 38, 313.

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UNIVERSITÉ DE STRASBOURG

14h30-15h00

Luminescence of lanthanide coordination polymers triggered by mechanical stimulation Yuichi Hirai,^a Yuichi Kitagawa,^b Takayuki Nakanishi,^c Koji Fushimi,^b Yasuchika Hasegawa^{b*} ^a PPSM ENS Cachan, CNRS, Université Paris-Saclay, 61 Avenue du Président Wilson, 94230, Cachan, France ^b Graduate School of Engineering, Hokkaido University, Kita 13-Jo Nishi 8-Chome, Kita-ku, Sapporo, 060-8628, Japan ^c Faculty of Industrial Science and Technology, Tokyo University of Science, 6-3-1, Niijuku, Katsushika-ku, Tokyo, 125-8585, Japan hasegaway@eng.hokudai.ac.jp

furan bridge

Triboluminescence (TL) is generally observed when crystalline inorganic, organic, and coordination compounds are mechanically stimulated. TL properties have been compared with those of photoluminescence (PL) to discuss the excitation, energy transfer, and emission mechanisms. In particular, lanthanide(III) coordination compounds are known to exhibit strong TL/PL properties.[1] We recently reported efficient PL lanthanide(III) coordination polymers with densely-packed structures,[2] and also designed specific facet-to-face molecular arrangements to introduce mechanically fragile structures for strong TL as well.[3] The prepared Eu(III) coordination polymers linked by furan-, edot-, or thiophene-based bridges showed characteristic red TL and PL. According to the single crystal X-ray analyses, the TL intensity was strongly related to the intermolecular arrangement of CF₃ groups, rather than the PL efficiencies excited by organic antenna ligands (Figure). We also found the first example of large TL/PL spectral difference. These results indicated that TL of lanthanide(III) coordination polymers would be generated through both organic ligands and lanthanide(III) ions.

edot bridge

thiophene bridge

Figure (top) TL pictures and spectra, and (bottom) corresponding intermolecular crystal structures of Eu(III) coordination polymers.

- 1. J.C.G. Bünzli, et al., J. Rare Earths, 2018, 36, 1.
- 2. Y. Hirai, Y Hasegawa, et al., Angew. Chem. Int. Ed., 2016, 55, 12059.
- 3. Y. Hirai, Y Hasegawa, et al., Angew. Chem. Int. Ed., 2017, 56, 7171.





15h00-15h30

ASSEMBLING MOLECULAR CRYSTALS

Sylvie FERLAY

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The design of complex molecular systems in the crystalline phase may lead to the development of new solid-state materials and devices. The fabrication of such networks of crystals displaying task-specific properties is a step toward smart molecular materials.

We have developed a strategy based on the formation of molecular core-shell crystals, using series of isostructural compounds, build either from H bonds¹ or coordination bonds.² entities.

A step further was reached by the welding, through 3D epitaxial growth, of iso-structural and almost iso-metric crystals into networks of crystals. Upon combining dicationic H-bond donor moities with anionic H-bond acceptor $[M^{II}L_2]^{4-}$ (M = Mn, Fe, Co, Ni, Cu or Zn) a series of iso-structural H-bonded robust coloured molecular crystals have been obtained.³ These compounds, characterized by XRD methods, are described as H-bonded 3D networks of formula 1₂-ML₂. Taking advantage of their isostructurality and difference in colour, different crystals have been welded in solution by epitaxial growth of a crystalline region between two seed crystals (figure 1).

More sophisticated monocrystals, presenting the control of the crystalline sequences along one axis, have been obtained by combining welding and also core-shell crystals.⁴

Crystal welding together with molecular core-shell crystals may be regarded as a first step toward the design of new hierarchically organized complex crystalline systems.

(i) (ii) (iii) Figure 1: Schematic representation (i), seed and welded crystals

pictures (ii) and welding from core-shell crystals (ii).

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- 2. F. Zhang, C. R. R. Adolf, N. Zigon, S. Ferlay, N. Kyritsakas, M. W. Hosseini Chem. Commun. 2017, 53, 3587.
- 3. C. R. R. Adolf, S. Ferlay, N. Kyritsakas, M. W. Hosseini J. Am. Chem. Soc. 2015, 137, 15390.
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16h00-16h30

Supramolecular oscillations and waves

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Looking at nature, we see that living materials with biological functionality, such as the actin or microtubule (MT) cytoskeletal network, achieve dynamics as well as supramolecular structures with the same protein building blocks. In other words, the components can assemble, but also react (i.e., tubulin is also an enzyme that hydrolyses guanosine triphosphate GTP), which in turn affects the assemblies. In this way, living systems create a built-in chemomechanical interaction. Moreover, such networks operate at the onset of oscillations,¹⁻³ which results in rapid response and adaptivity. In the case of MTs, oscillations stem from auto-amplification of MT production by higher concentrations of MTs due to their nucleation-elongation self-assembly mechanism.⁴ Negative (delayed) feedback comes from GTP to GDP hydrolysis that creates mechanical stress build-up in the MT leading to sudden bursting called "catastrophes". Here, we present an artificial supramolecular polymer that shows oscillations in a semi-batch reactor.⁵ The system is based on redox switching of the monomer between an assembled and disassembled state using

chemical fuels. In spatially extended systems waves and patterns are observed. Dissipative structures in the Prigogine-sense can be made in this way, where self-assembly is coupled to large scale transport phenomena.

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2. Valiron, O., Caudron, N. & Job, D. Microtubule dynamics. Cell. Mol. Life Sci. CMLS *58*, 2069–2084 (2001).

3. Westendorf, C. et al. Actin cytoskeleton of chemotactic amoebae operates close to the onset of oscillations. Proc. Natl. Acad. Sci. *110*, 3853–3858 (2013).

4. Lange, G., Mandelkow, E.-M., Jagla, A. & Mandelkow, E. Tubulin oligomers and microtubule oscillations. Eur. J. Biochem. *178*, 61–69 (1988).

5. Leira-Iglesias, J., Stich, M., Hermans, T.M., under review (2018)





16h30-17h00

Single-Molecule Level Analysis of DNA by Controlling the Fluorescence Blinking

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In order to achieve a ultra-sensitive analysis, one strategy would be to focus on an analytic method that relies on the properties of molecules that become highlighted when we look at molecules at the single-molecule level. Herein, we focused on the phenomenon so called fluorescence blinking. Fluorescent signals from a single fluorophore often blink, reflecting time-dependent fluctuations between bright "ON" and dark "OFF" states. During the repetitive cycles of excitation and emission, fluorescent molecules may occasionally enter non-fluorescent off states, such as a triplet state, a radical ion state, and an isomerized state. Reversible formation of such off states causes a fluorescence blinking. The kinetics of a reaction concomitant with blinking can be followed by the duration of the ON state (τ_{ON}) and that of the OFF state (τ_{OFF}). Based on the understanding of factors that affect the blinking, single fluorescent molecules can serve as reporters of their local microenvironment. We developed a method, termed Kinetic Analysis based on the Control of fluorescence Blinking (KACB). The blinking kinetics or patterns were controlled to reflect the microenvironment changes around the fluorophore. In this study, KACB method was adapted for analysis of DNA structures such as a single strand, a hairpin, a duplex, and a triplex, and for investigation of antigenantibody interactions at the single molecule level.



Figure Schematic representation of KACB method.

- 1. T. Miyata, N. Shimada, A. Maruyama, K. Kawai, *Chem. Eur-J.*, **2018**, *24*, 6755.
- 2. K. Kawai, T. Miyata, N. Shimada, S. Ito, H. Miyasaka, A. Maruyama, *Angew. Chem. Int. Ed.* **2017**, *56*, 15329.
- 3. K. Kawai, A. Maruyama, Chem. Commun. 2015, 51, 4861.

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THE SATELLITE INTERNATIONAL SYMPOSIUM ON SOFT CRYSTALS IN EUROPE, 5 JULY, 2018, STRASBOURG, FRANCE

17h00-17h30

New twist on light-matter interactions: the role of chirality

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Artifical chiral nanostructures have opened new perspectives in the field of colloidal science, optics, and spectroscopy [1]. Chiral plasmonic nanostructures, for instance, have led to the possibility of enhancing chiroptical signals through the excitation of so-called superchiral electromagnetic fields [2-3]. Such progress have also renewed with fundamental questions related to the role played by the concept of chirality in light-matter interactions. This is particularly true role in relation to light-induced motional effects. New predictions have been given recently, showing in particular how chiral light modes can exert genuinely new optical forces on chiral objects [4]. Because directly connected to standard chiroptical molecular observables (rotatory power or circular dichroism, e.g.) such new chiral optical forces become enantiomer-dependent. The general framework of the context will be sketched before discussing possible strategies for manipulating, recognizing and separating chiral matter at the nanoscale [5].



Figure Far-field optical vortices generated from spin-orbit coupling on a chiral plasmonic nanostructure [3].

- 1. A. Ben-Moshe, B.M. Maoz, A.O. Govorov, and G. Markovich, *Chem. Soc. Rev.*, **2013**, 42, 7028.
- 2. S. Boriskina and N.I. Zheludev, Singular and Chiral Nanoplasmonics (CRC Press 2014).
- 3. Y. Gorodetski, A. Drezet, C. Genet, and T.W. Ebbesen, *Phys. Rev. Lett.* **2013**, 110, 203906.
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- 5. G. Schnoering, et al., Phys. Rev. Lett. 2018, Accepted.





17h30-18h00

The potential of lanthanide luminescence for MOFs and SURMOFs

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The potential of lanthanide coordination compounds in biological and lighting applications can hardly be overestimated due to their fascinating optical properties. They exhibit sharp, nonoverlapping, and easily identifiable emission bands in both the visible and NIR [1].

Metal-organic frameworks (MOFs) are solid crystalline cooridination materials which hold great promise for a variety of applications including gas storage, chemical separation, catalysis, sensing, and fuel cells [2]. Due to their high crystallinity and tunable pore size as well as the possibility of incorporation of various functionalities via linker modification, they are recognized as a perspective hosting material for many guest species including enzymes, nanoparticles, dyes and lanthanide cations. Moreover the use of lanthanide ions as MOFs nodes has been demonstrated [3].

Unlike lanthanide-doped nanocrystals, lanthanide-based MOFs have easily characterizable crystalline structures, allowing the reproducible formation of the materials and, therefore, control on their luminescent properties on the basis of its structure [1].

For several advanced application, especially where the thin films or layered structure of material are needed, the surface mounted MOFs (SURMOFs) can be obtained. We and others have already shown that the SURMOFs have wide range of applications [2,4,5]. In this regards, the combination of great promise of SURMOF with our broad experience in the lanthanide complexes allow creation of perspective new materials for medicine, sensing and optoelectronics [6].



Figure (a) emission of Eu(III) complex (left) and Tb(III) complex (right), and (b) representation of SURMOF structure.

- 1. K.A. White, et al. *JACS* **2009**, 131, 18069.
- 2. *The Chemistry of Metal-Organic Frameworks* by S. Kaskel, Wiley-VCH, **2016**.

3. H. Liu, et al, *J. Mater. Chem. C* **2014**, 2, 8683-8690; Y. Cui, et al. *JACS* **2012**, 134, 3979.

- 4. S. Bräse, C. Wöll, et al. ACS Nano 2014, 8, 1463-1467
- 5. S. Bräse, C. Wöll, M. Tsotsalas, et al. *Chem. Materials A* 2016, *4*, 6815.
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The Satellite Symposium on **Soft Crystals**

The 7th International Mini-symposium on Advanced Coordination Chemistry

We thank Madame Valérie Rey (U. Strasbourg) and the members of Prof. Hosseini group.

Organizing committee members: Miki Hasegawa (Aoyama Gakuin U.) Mia Wais Hosseini (U. Strasbourg) Hitoshi Goto (Toyohashi U. of Tech.)

29 June, 2018