3-dimensional topology and polycontinuous pattern

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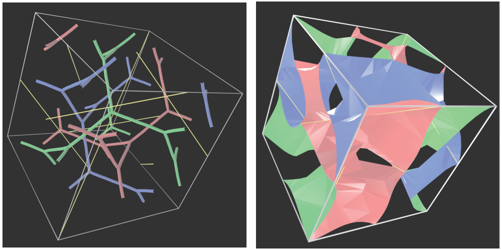
The Topology of Nucleic Acids:
Research at the Interface of Low-Dimensional Topology,
Polymer Physics and Molecular Biology
March 26, 2019

Banff International Research Station for Mathematical Innovation and Discovery

Discrete Geometric
Analysis for
Materials Design

Block copolymer and microphase-separated structure, 3D network, and handlebody decomposition of 3-manifolds



K.Ishihara, Y.Koda, M.Ozawa, and K.Shimokawa,

Topology Appl **257** (2019) 11-21.

Metal-peptide rings form highly entangled topologically inequivalent frameworks with the same ring- and crossing-numbers

ring number (n):	4	4
crossing number (c):	12	12
name:	T_2-tetrahedral link	three-crossed tetrahedral link
diagram:		

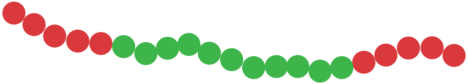
T.Sawada, A.Saito, K.Tamiya, K.Shimokawa, Y.Hisada, and M.Fujita,

Nature Communications **10**, Article number: 921 (2019)

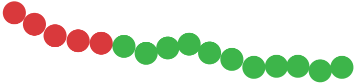
Block copolymer and microphase-separated structure

Block copolymer

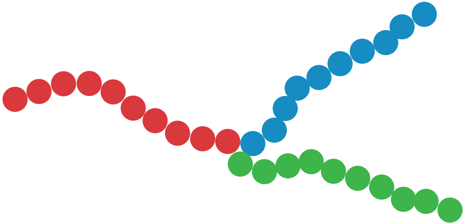
ABA type triblock copolymer



AB type diblock copolymer



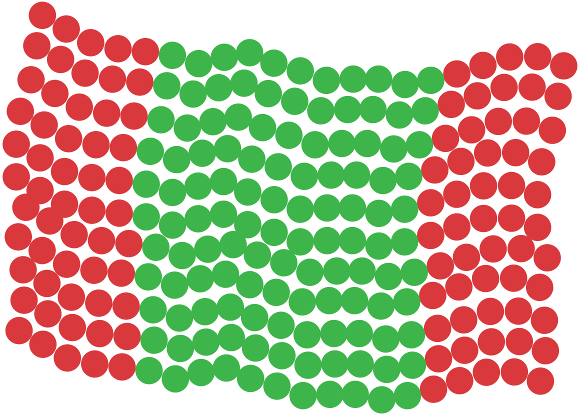
ABC type triblock copolymer



Ex. hydrophilic, fluorophilic, oleophilic

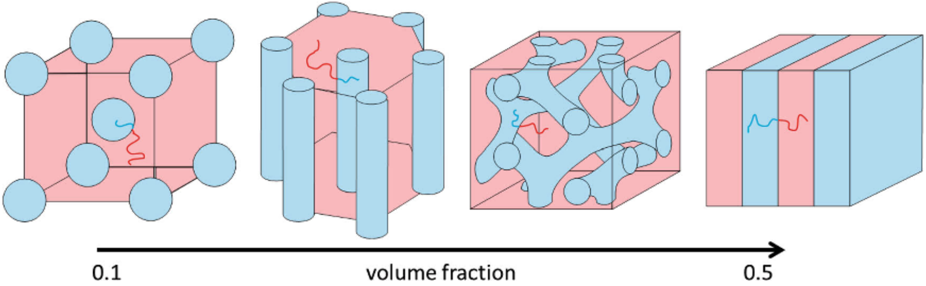
Microphase-separated structure

Microphase-separated structure of ABA type triblock copolymer



Microphase-separated structure

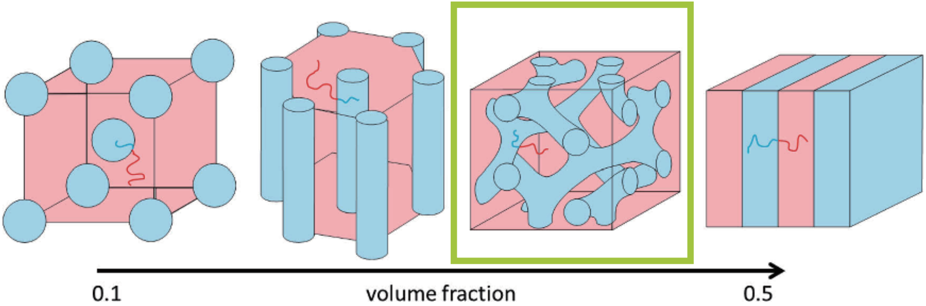
Microphase-separated structure of block copolymer



V. Abetz, Macromolecular rapid communications (2015)

Microphase-separated structure

Microphase-separated structure of block copolymer



V. Abetz, Macromolecular rapid communications (2015)

Here we will consider poly-continuous structure

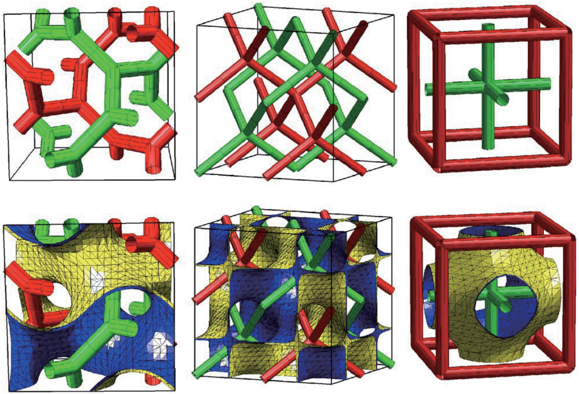
Bicontinuous structure

Bicontinuous structure

Definition

Bicontinuous pattern is a 3-periodic surface that divides $\mathbb{R}^3$ into two 3-periodic labyrinths (domains).

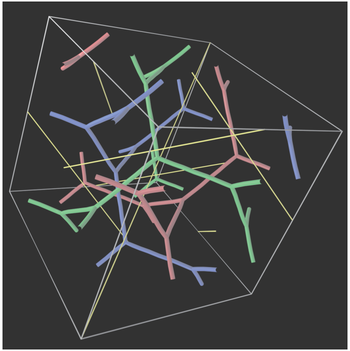
Spines of labyrinths form interwoven networks.

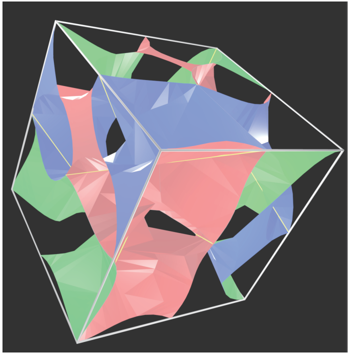


Tricontinuous structure

Definition

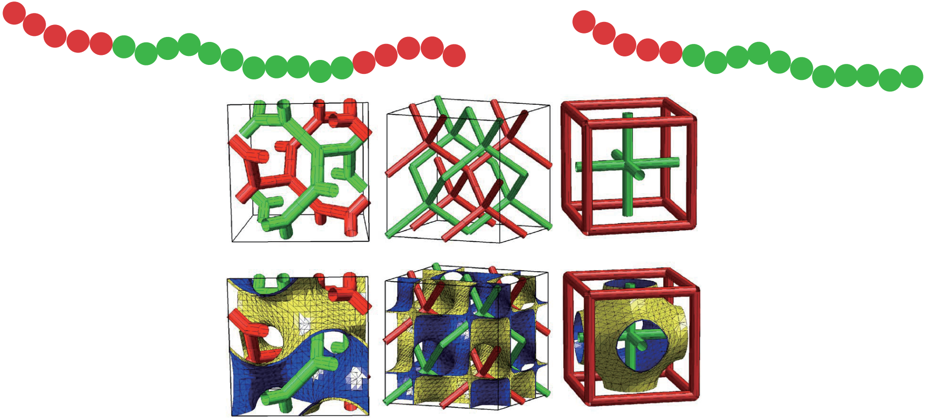
Tricontinuous pattern is a 3-periodic branched surface that divides $\mathbb{R}^3$ into three 3-periodic labyrinth.





Entangled networks and bicontinuous pattern

ABA type triblock copolymer AB type diblock copolymer

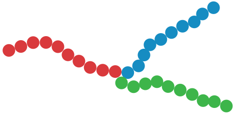


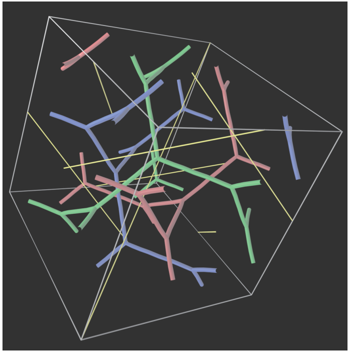
SQUIRES et al., Phys. Rev. E 72, 011502 (2005)

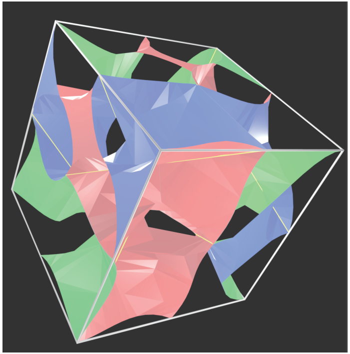
Entangled networks and triply periodic bicontinuous pattern

Entangling of 3 networks and tricontinuous pattern

ABC type triblock copolymer



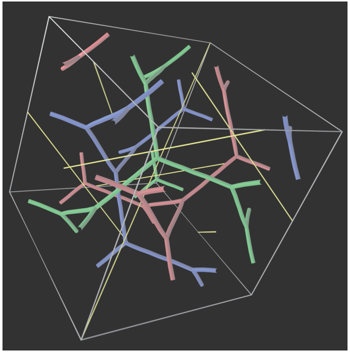


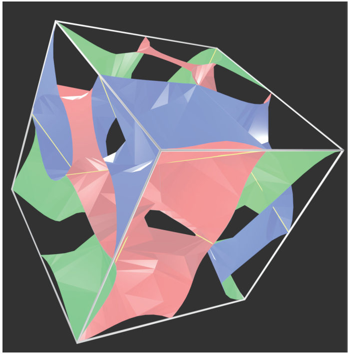


Bicontinuous pattern and topology

One goal

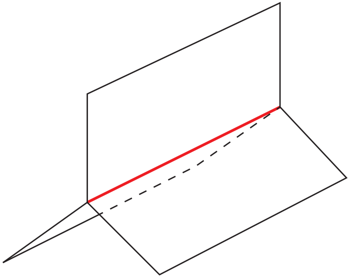
- Topological classification of poly-continuous pattern
- Characterization of poly-continuous pattern using topological invariants





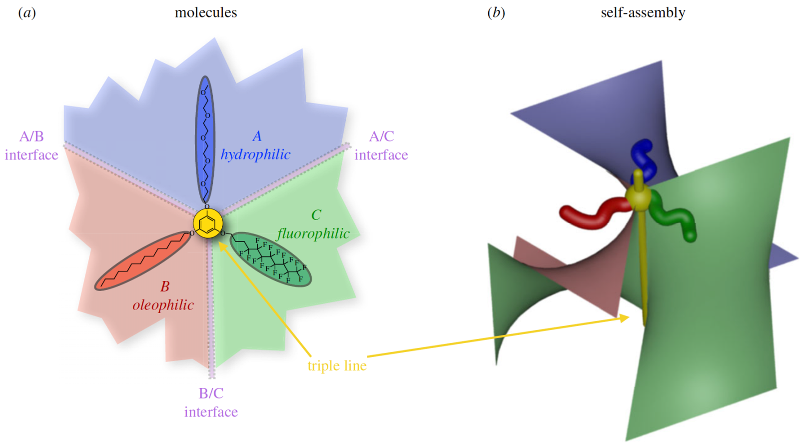
Tribranch surface

Here we use tribranched surface for tricontinuous pattern.



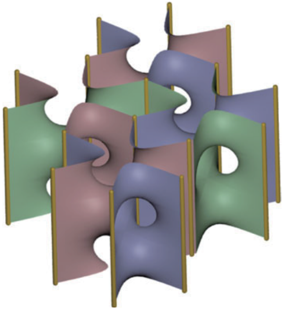
Red line is a branch locus.

Tricontinuous pattern

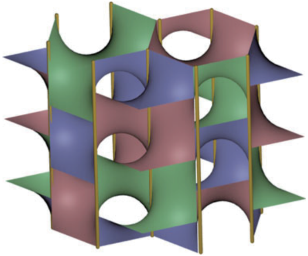


de Campo L, Castle T, Hyde ST. (2017) Interface Focus 7: 20160130.

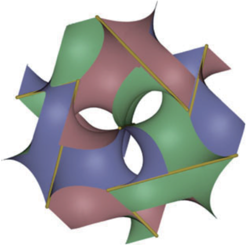
Tricontinuous pattern



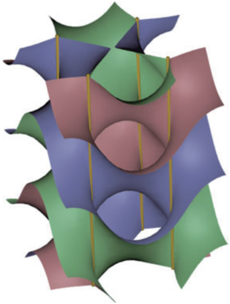
3etc



3pcu



3srs



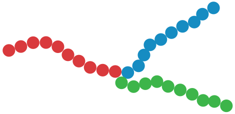
3dia

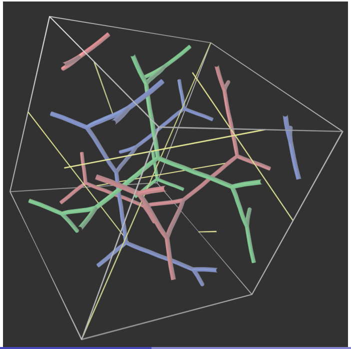
de Campo L, Castle T, Hyde ST. (2017) Interface Focus 7: 20160130.

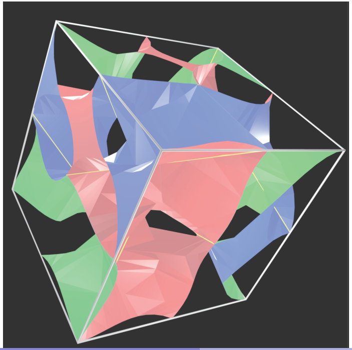
Poly-continuous pattern and network

Entangling of 3 networks and tricontinuous pattern

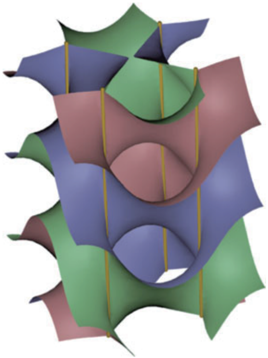
Poly-continuous pattern and network

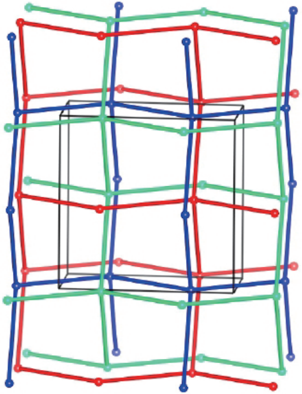






Tricontinuous pattern



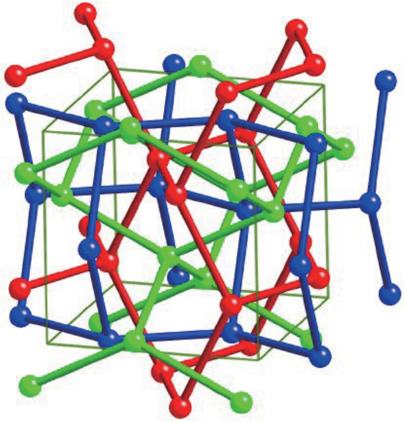


3dia (dia-c3*)

de Campo L, Castle T, Hyde ST. (2017) Interface Focus 7: 20160130.

RCSR reference: http://rcsr.net/nets/dia-c3*

dia-c3

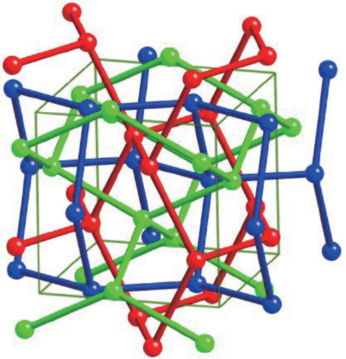


3dia (dia-c3)

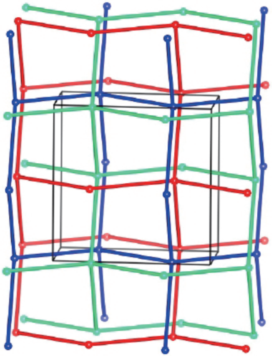
de Campo L, Castle T, Hyde ST. (2017) Interface Focus 7: 20160130.

RCSR reference: http://rcsr.net/nets/dia-c3

two 3dia networks



3dia (dia-c3)

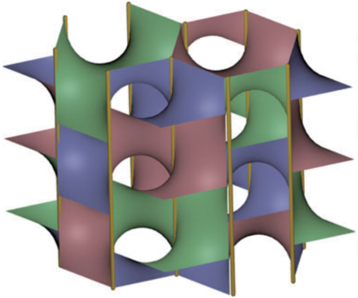
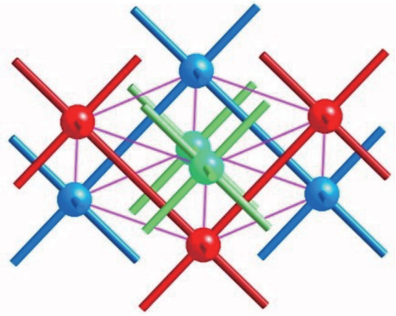


3dia (dia-c3*)

Problem

How can we characterize tricontinuous pattern?

Tricontinuous pattern

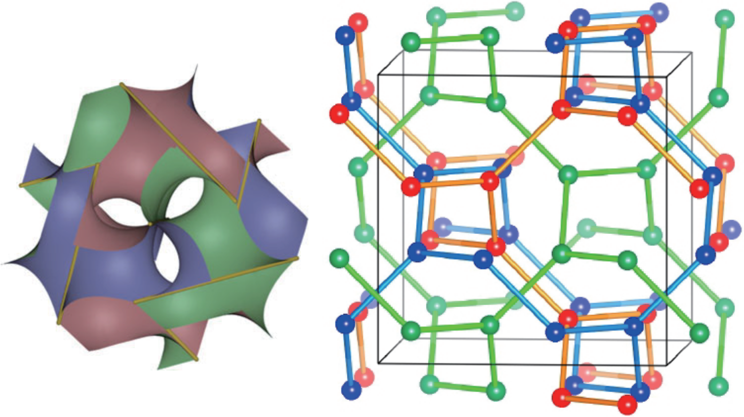



3pcu

de Campo L, Castle T, Hyde ST. (2017) Interface Focus 7: 20160130

RCSR reference: http://rcsr.net/nets/pcu-c3

Tricontinuous pattern

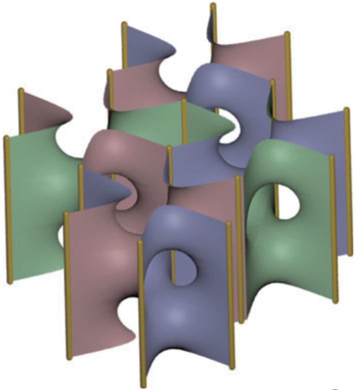


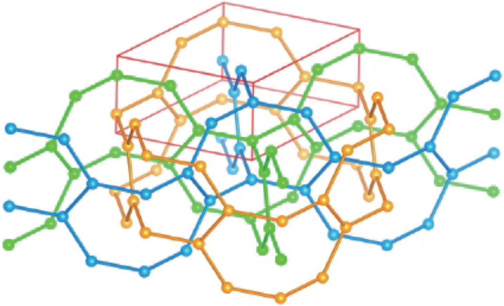
3srs

(three K_4 lattice)

de Campo L, Castle T, Hyde ST. (2017) Interface Focus 7: 20160130, RCSR reference: http://rcsr.net/nets/srs-c3

Tricontinuous pattern





3etc

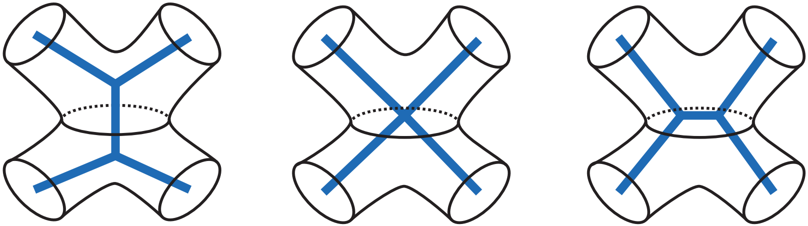
RCSR reference: http://rcsr.net/nets/etc-c3

Entangled networks and bicontinuous pattern

Networks and bicontiuous patterns

Observation

- Network determines bicontinuous pattern uniquely
- Bicontiuous pattern determines network up to IX-XI moves



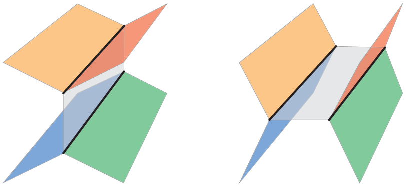
IX-XI move of networks

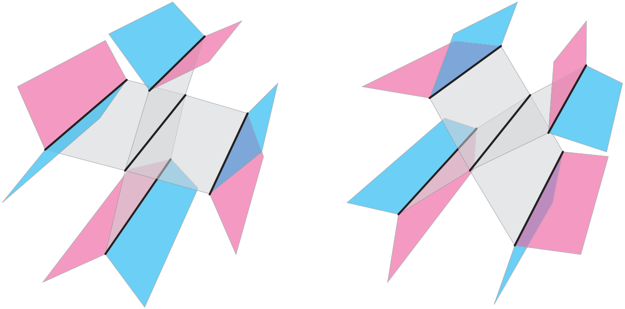
Entangled network and tricontinuous pattern

We consider entangled networks with 3 components and tricontinuous patterns

Thm(Ishihara-Koda-Ozawa-S, Topology Appl (2019))

There is one-to-one correspondence between entangled networks with 3 components and tricontinuous pattern up to IX-XI moves of networks and tribranched surfaces.





Entangled network and tricontinuous pattern

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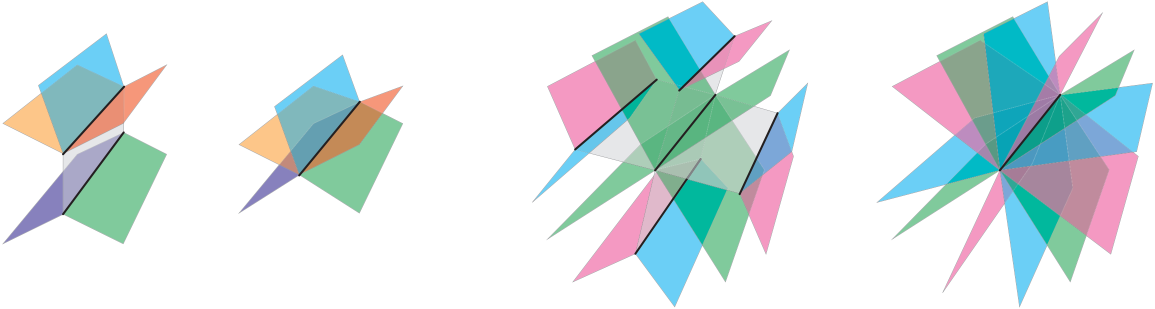


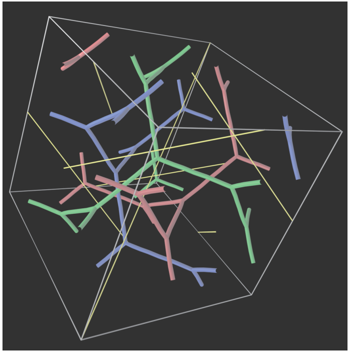
Corollary

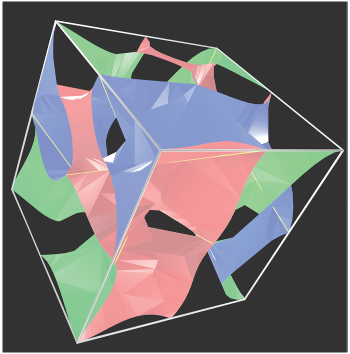
We can study tricontinuous pattern using networks.

Entangled network and tricontinuous pattern

Thm(Ishihara-Koda-Ozawa-S, Topology Appl (2019))

There is one-to-one correspondence between entangled networks with 3 components and tricontinuous pattern up to IX-XI moves of networks and tribranched surfaces.

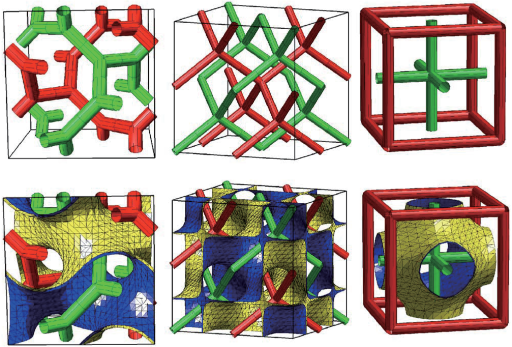


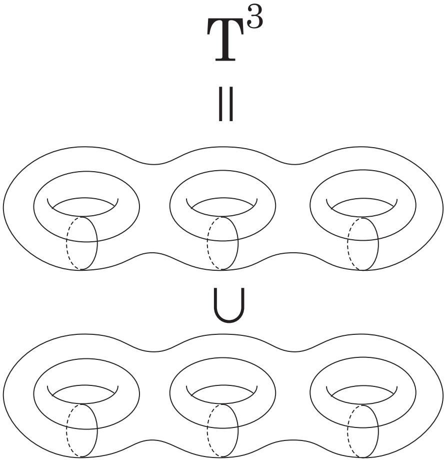


3-dimensional torus and poly-continuous pattern

Bicontinuous structure and Heegaard splittings

Triply periodic bicontinuous structure corresponds to a Heegaard splitting of the 3-dimensional torus $T^3 = S^1 \times S^1 \times S^1 = \mathbb{R}^3/\mathbb{Z}^3$.

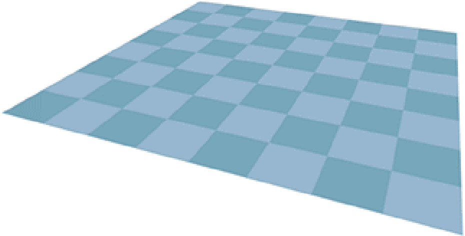




SQUIRES et al., Phys. Rev. E 72, 011502 (2005)

2-dimensional torus

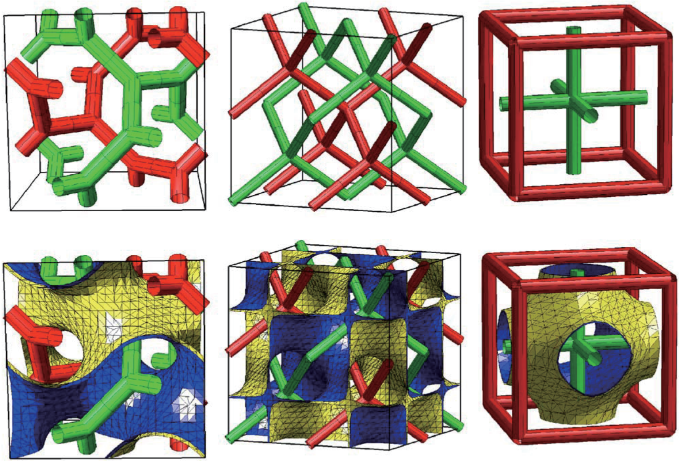
2-dimensional torus $\boldsymbol{T^2} = \boldsymbol{S^1} \times \boldsymbol{S^1} = \mathbb{R}^{\mathbf{2}}/\mathbb{Z}^{\mathbf{2}}$



(wikipedia "Torus")

3-dimensional torus

3-dimensional torus $T^3 = S^1 \times S^1 \times S^1 = \mathbb{R}^3/\mathbb{Z}^3$

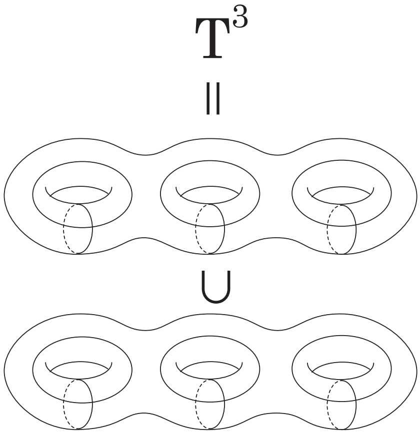


Heegaard splittings

Definition

M : closed orientable 3-manifolds
H_i : handlebody
$M = H_1 \cup H_2$: Heegaard splitting
$\Leftrightarrow H_1 \cap H_2 = \partial H_1 \cap \partial H_2 = S$

Genus 3 Heegaard splitting of T^3



Heegaard splitting of T^3

Theorem[Frohman-Hass, Invent. Math. 1989]

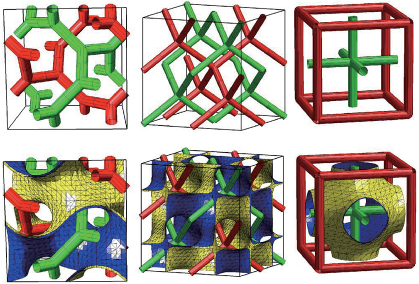
Genus 3 Heegaard splitting of T^3 is unique up to homeomorphism.

Theorem[Boileau-Otal, JDG 1990]

Genus n Heegaard splitting of T^3 is unique up to homeomorphism.

Frohman-Hass theorem is proved by using minimal surfaces.

These theorem will give information of bicontinuous structure.



SQUIRES et al., Phys. Rev. E 72, 011502 (2005)

Handlebody decomposition

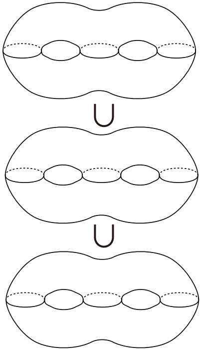
Definition

M : closed orientable 3-manifolds
H_i : handlebody
$M = H_1 \cup H_2 \cup H_3$: handlebody decomposition
$\Leftrightarrow H_i \cap H_j = \partial H_i \cap \partial H_j$ is a compact surface (possibly disconnected)

$B = \partial H_1 \cup \partial H_2 \cup H_3$
is a tribranch surface.
If each $H_i \cap H_j$ is connected,
this is called a trisection of
a 3-manifold.

Example of type $(2, 2, 2)$ handlebody decomposition

$T^3 =$



Handlebody decomposition

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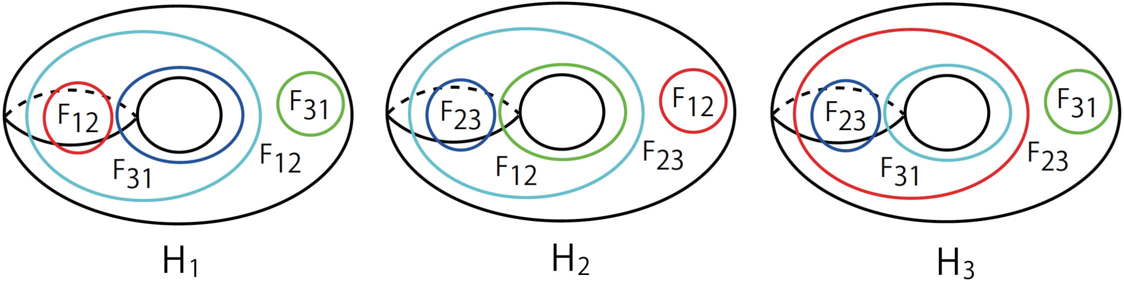


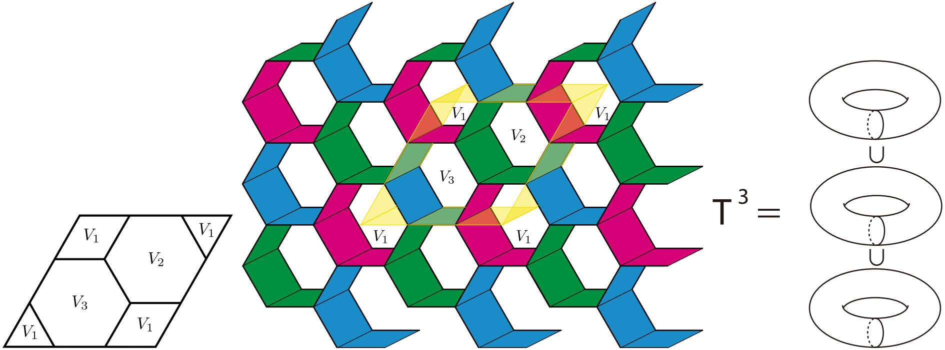
Problem

Problem

Characterize handlebody decompositions of T^3.

Theorem (Ishihara-Koda-Ozawa-Sakata-S)

Type $(1, 1, 1)$ handlebody decomposition of T^3 that corresponds to the honeycomb pattern.

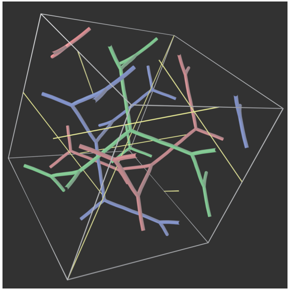


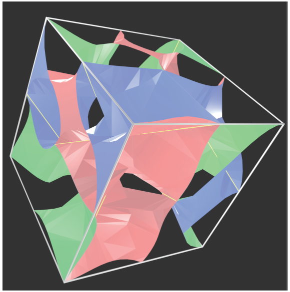
Problem

Problem

Characterize handlebody decompositions of T^3.

Characterization of type $(3,3,3)$ (or (n,n,n)) handlebody decomposition will give a characterization of tricontinuous patterns.





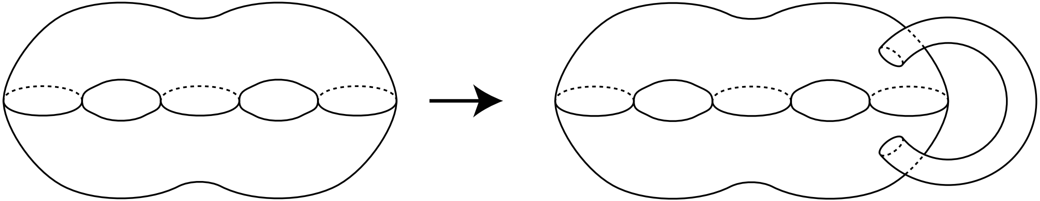
Stabilization theorem

Stably equivalence of Heegaard splitting

Reidemeister-Singer Theorem

Any two Heegaard splittings of a 3-manifold are stably equivalent.
That is, sequence of stabilizations yields equivalent Heegaard splittings.

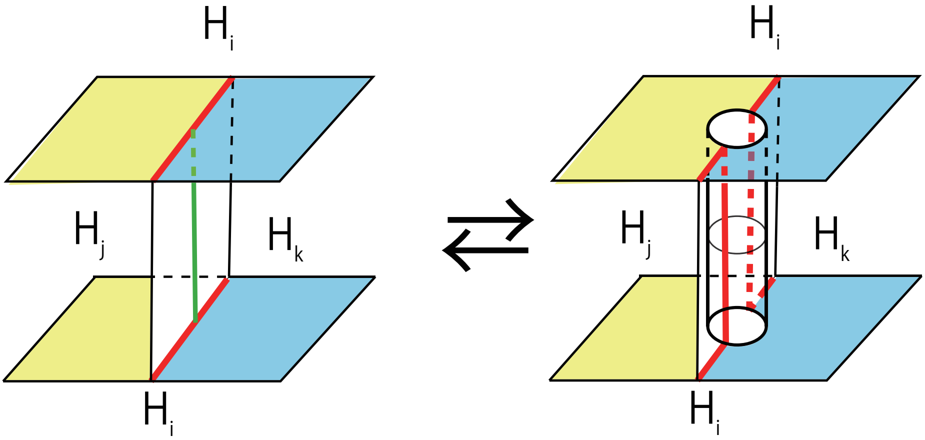
We will generalize this.



Stabilization of a Heegaard splitting

Stabilization of handlebody decomposition

Stabilization yields another handlebody decomposition.

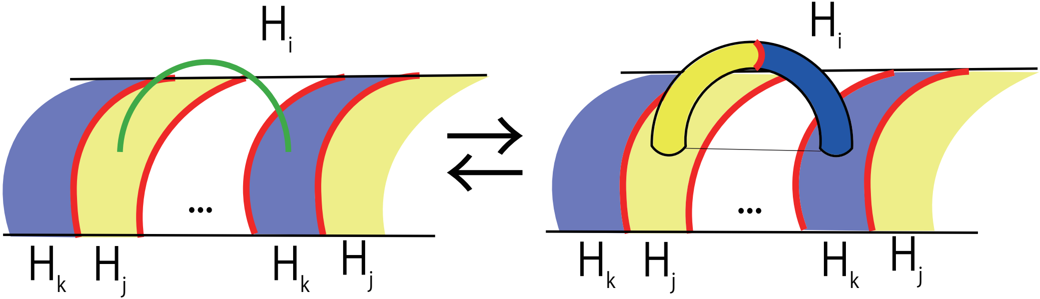


Stabilization of type Ia

Stabilization yields new complex tricontinuous structure from simple one.

Stabilization of handlebody decomposition

Stabilization yields another handlebody decomposition.

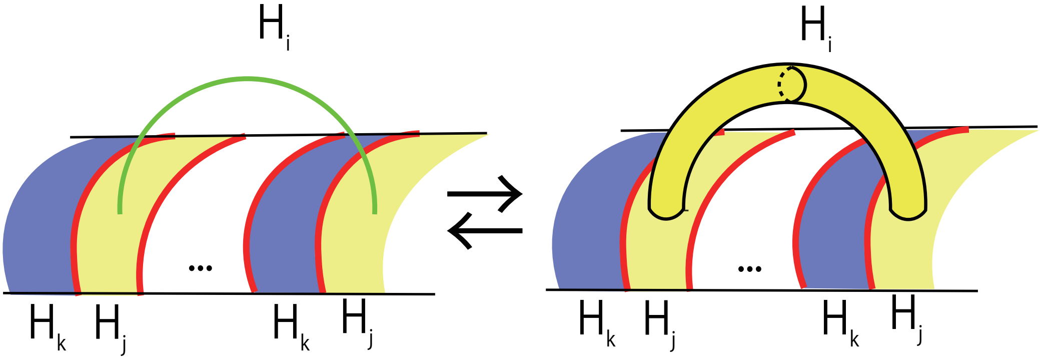


Stabilization of type Ib

Stabilization yields new complex tricontinuous structure from simple one.

Stabilization of handlebody decomposition

Stabilization yields another handlebody decomposition.



Stabilization of type II

Stabilization yields new complex tricontinuous structure from simple one.

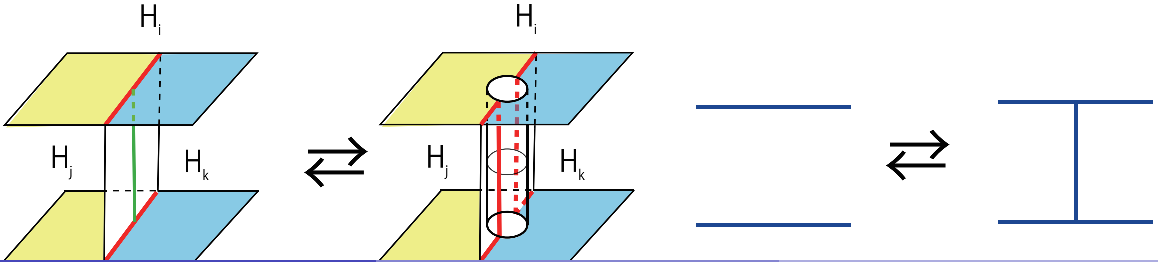
Stably equivalence of handlebody decomposition

Stably equivalence theorem (Koenig, Ishihara-Ito-Koda-Ozawa-S 2018)

Two decompositions of a 3-manifold with 3 handlebodies are stably equivalent.
That is, a sequence of stabilizations and destabilization yields equivalent handlebody decompositions.

Cororally

We can relate one tricontinuous structure with another by a sequence of stabilization, destabilization and homeomophisms.



Stably equivalence of handlebody decomposition

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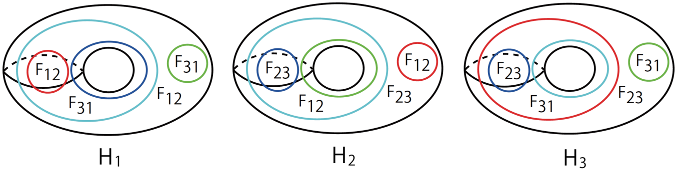
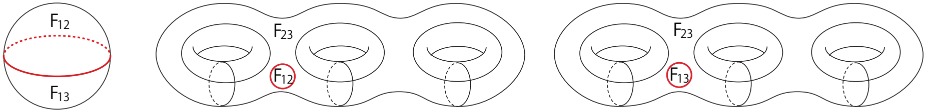


$(g_1, g_2, g_3; b)$



$(0, g, g; 1)$

Non-stabilized decomposition

Theorem [Boileau-Otal 1990]

Any Heegaard splitting of $\boldsymbol{T^3}$ with genus at least 4 is stabilized.

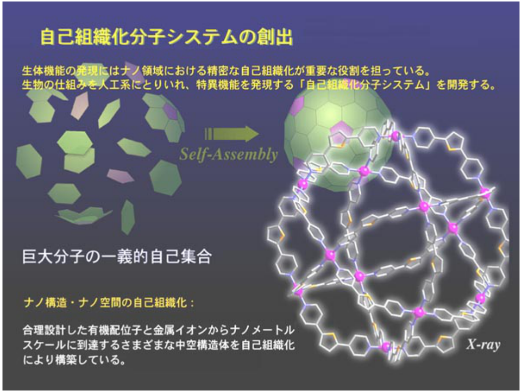
Theorem [Mishina 2019]

- No type $(\mathbf{0}, \mathbf{0}, \mathbf{3})$ decomposition of $\boldsymbol{T^3}$ is stabilized.
- No type $(\mathbf{0}, \mathbf{2}, \mathbf{2})$ decomposition of $\boldsymbol{T^3}$ is stabilized.
- No type $(\mathbf{1}, \mathbf{1}, \mathbf{1})$ decomposition of $\boldsymbol{T^3}$ is stabilized.

§2 Metal-peptide rings form highly entangled topologically inequivalent frameworks with the same ring- and crossing-numbers

Self-assembly

Self-assembly of molecular polyhedra



Fujita lab homepage (http://fujitalab.t.u-tokyo.ac.jp)

12-crossing peptide [4]catenanes

Metal-peptide rings form highly entangled topologically inequivalent frameworks with the same ring- and crossing-numbers

T.Sawada, A.Saito, K.Tamiya, K.Shimokawa, Y.Hisada, and M.Fujita,

Nature Communications **10**, Article number: 921 (2019)

Selective construction of two topologies of 12-crossing peptide [4]catenanes from metal ions and pyridineappended tripeptide ligands.

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ARTICLE

https://doi.org/10.1038/s41467-019-08879-7 OPEN

Metal–peptide rings form highly entangled topologically inequivalent frameworks with the same ring- and crossing-numbers

Tomohisa Sawada[1], Ami Saito[1], Kenki Tamiya[1], Koya Shimokawa[2], Yutaro Hisada[1] & Makoto Fujita[1]

With increasing ring-crossing number (c), knot theory predicts an exponential increase in the number of topologically different links of these interlocking structures, even for structures with the same ring number (n) and c. Here, we report the selective construction of two topologies of 12-crossing peptide [4]catenanes ($n = 4$, $c = 12$) from metal ions and pyridine-appended tripeptide ligands. Two of the 100 possible topologies for this structure are selectively created from related ligands in which only the tripeptide sequence is changed: one catenane has a T_2-tetrahedral link and the other a three-crossed tetrahedral link. Crystallographic studies illustrate that a conformational difference in only one of the three peptide residues in the ligand causes the change in the structure of the final tetrahedral link. Our results thus reveal that peptide-based folding and assembly can be used for the facile bottom-up construction of 3D molecular objects containing polyhedral links.

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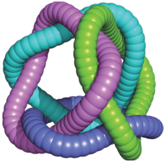
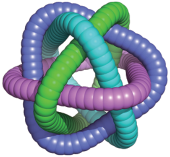
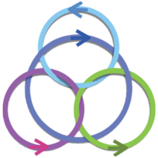
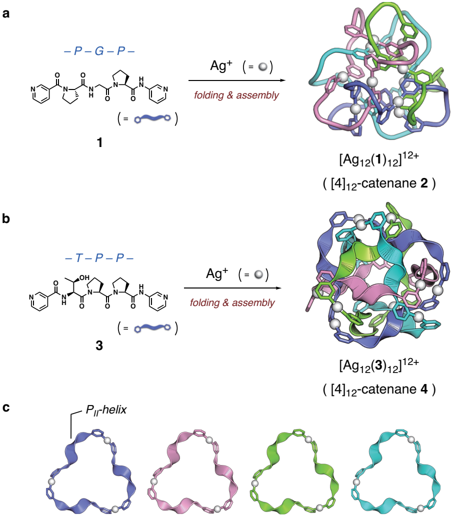
12-crossing peptide [4]catenanes

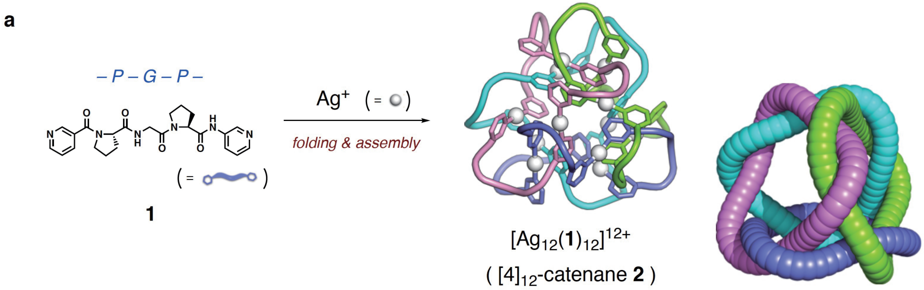
		
ring number (n):	4	4
crossing number (c):	12	12
name:	T_2-tetrahedral link	three-crossed tetrahedral link
diagram:		

12-crossing peptide [4]catenanes



P: L-proline
G: glycine
T: L-threonine

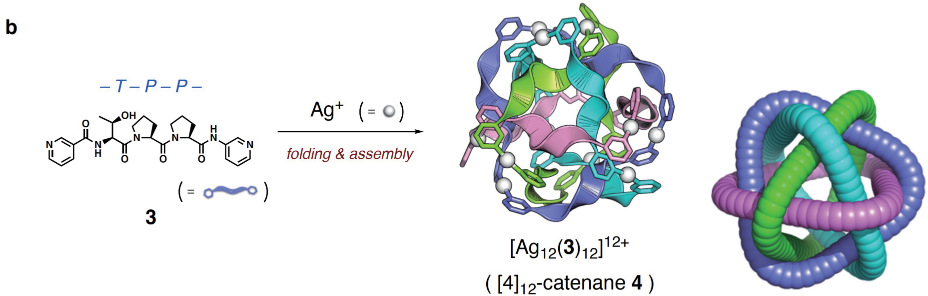
12-crossing peptide [4]catenanes



P: L-proline, G: glycine

12-crossing peptide [4]catenanes from metal ions and pyridineappended tripeptide ligands

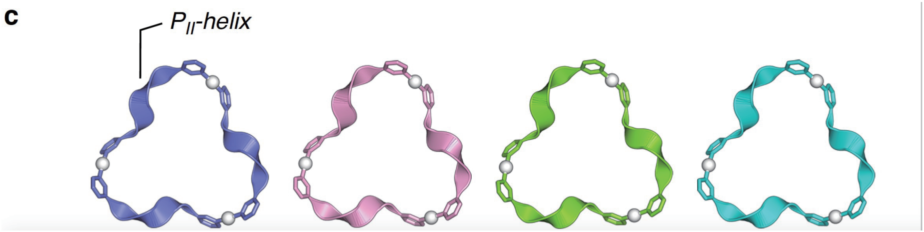
12-crossing peptide [4]catenanes



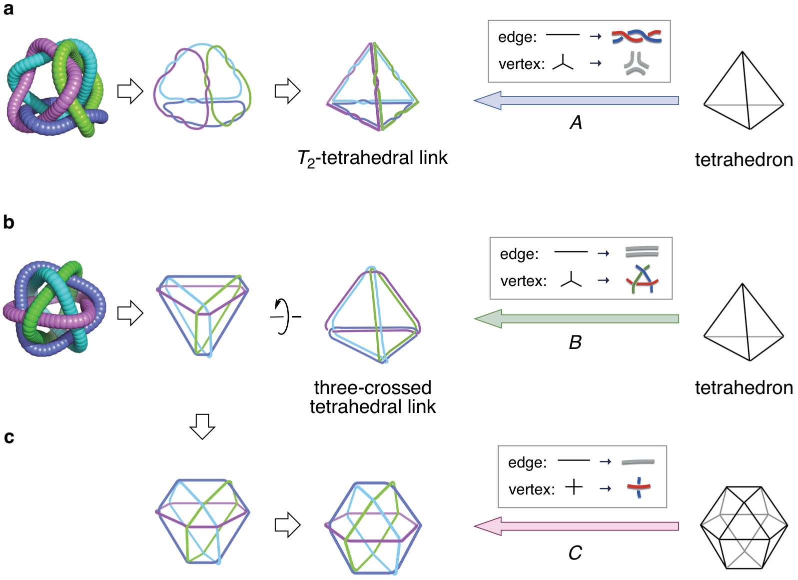
P: L-proline, T: L-threonine

12-crossing peptide [4]catenanes from metal ions and pyridineappended tripeptide ligands

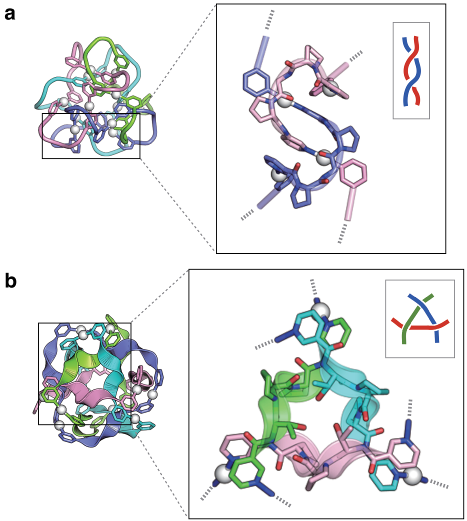
12-crossing peptide [4]catenanes



12-crossing peptide [4]catenanes

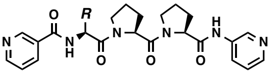


12-crossing peptide [4]catenanes



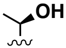
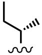
12-crossing peptide [4]catenanes

– X – P – P –



Ag^+ → *folding & assembly*

a single topology of the $[4]_{12}$-catenane

	peptide sequence	-R	$[4]_{12}$-catenane type
3	*– T – P – P –*		*three-crossed tetrahedral link*
5	*– A – P – P –*		*three-crossed tetrahedral link*
6	*– I – P – P –*		*T_2-tetrahedral link*
7	*– V – P – P –*		*T_2-tetrahedral link*

Conlcusion

- Microphase-separated structure of block copolymer can be studied using 3-dimensional topology
- Relation between poly-continuous structure and entangled networks is given
- Characterization of handlebody decomposition of 3-dimensional torus gives characterization of poly-continuous structure
- Modification of poly-continuous structure into another is provided

- Self-assembly construction of 12-crossing peptide [4]catenanes from metal ions and pyridineappended tripeptide ligands

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- Makoto Ozawa (Komazawa U)
- Yuya Koda (Hiroshima U)
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- Makoto Fujita (U Tokyo)
- Tomohisa Sawada (U Tokyo)
- Ami Saito (U Tokyo)
- Yutaro Hisada (U Tokyo)

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戦略的創造研究推進事業 CREST

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