

# Alan Schoen 100th birth anniversary

## Gyroid is everywhere

Kindai, Osaka, 2024

<u>Date</u> November 19-22, 2024

Venue Kindai University

Organizers Alan Schoen 100th Birth Anniversary Organizing Committee

Photonic Structures On Th Of Butterflies, Beetles and

D.G. Stavenga Computational Physics University of Groningen the Netherlands

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Program and Abstracts for

## Gyroid is everywhere

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Toyota Physical and Chemical Research Institute





## Greeting

Alan Hugh Schoen was an American physicist and computer scientist renowned for his discovery of the gyroid, an infinitely connected triply periodic minimal surface. The gyroid discovered by Dr. Schoen is a structure seen in butterfly wings and the self-assembly of lipids, surfactants, and polymers, and it is studied in a wide range of fields including mathematics, physics, chemistry, biology, materials science, mechanical engineering, and medicine.

He was born on December 11, 1924, in Mount Vernon, New York. After graduating from Yale University, he came to Japan with the Occupation Forces. After returning to the United States, he earned a Ph.D. in physics from the University of Illinois and later taught at Niigata campus of Southern Illinois University. Unfortunately, he passed away on July 26, 2023, in Carbondale, Illinois, United States † .

In commemoration of his 100th birth anniversary, we are organizing a symposium entitled "Alan Schoen 100th birth anniversary – Gyroid is everywhere" from November 19 to November 22, 2024, at Kindai University, Osaka, Japan. This symposium is made possible through the support of Toyota Riken, The Simons Foundation, and Kindai University.

The international symposium aims to achieve the following three objectives:

- 1) Discover gyroid in nature and create unconventional materials, exemplified by molecular gyroids.
- 2) Renovate existing soft gyroid research with unprecedented material design principles.
- 3) Discover the foundational principles (geometry and topology) and novel functionalities of gyroids, leading to a rapid transformation and innovation in the material science of gyroids.

By setting these three goals – creation of gyroid substances, renovation of traditional gyroid research, and transformation of gyroid science – the symposium seeks to bring together researchers who align with these objectives. The symposium serves as a starting point to foster future gyroid science. As one of the strategies for strategic international collaboration, the event aims to gather top-tier theoretical researchers in the field of natural sciences along with a diverse group of experimental researchers in science and engineering. Encouraging interaction, promoting interdisciplinary collaboration, and facilitating reorganization of international collaboration, the symposium aims to transform and advance gyroid research worldwide into a new dimension of comprehensive research areas.

<sup>†</sup> Stephen T. Hyde and Gerd E Schroeder-Turk, Physics Today, Jan. 2024.

#### Message from Reiko Shoen

I am delighted to congratulate you on the Gyroid Is Everywhere conference. I would like to express thanks from the bottom of my heart to the members of the conference committee, international advisers, Dr. Hyde, Dr. Kamien, Dr. Matsushita, Dr. Schröder-Turk and local organizers, Dr. Dotera, Dr. Takano, Dr. Ichikawa, and Dr. Sugahara for their efforts in organizing Alan Schoen 100<sup>th</sup> Anniversary conference.

I am grateful to all of you, the professors and the researchers from across the world for your contributions to Alan's legacy. I wish Alan could be here to meet with you.

On this occasion, I would like to share with you two videos. The link on left at the bottom contains a collection of minimal surface models and his puzzles made by Alan. The background piano music is Chopin's Nocturne in D-flat Major, Op. 27, No.2 played by me.

Recently I established a new Yellow Moon Gyroid concert series in the Southern Illinois University in the Morris library where Alan and I donated the Yellow Moon Gyroid sculpture in 2022. It was created by algorithmic artist Jesse Louis-Rosenberg, New York. This room became the place on campus where science, art, architecture, and music come together in harmony.

The link on the right below is the premier performing video of the commissioned composition for the opening gala concert in this series on September 19<sup>th</sup>, 2024. It is called "The Gyroid" by Thomas Edgar---the winner at the international Saint-Saëns Music competition in composition in 2024. He noted "In an effort to evoke this fascinating scientific phenomenon, I compositionally confined myself to a three-not intervallic structure which serves as the foundation for every developmental aspect of the music. My goal was to demonstrate the infinite nature and complexity of the gyroid's structure, all while using a minimal amount of constructional content.

He earned a bachelor's degree in May '24 in both piano performance and aviation flight at SIU. In this video he is on piano, and Iasmim Bonfim de Carvalho, a master student at SIU from Brazil, is playing Alan's violin, which I let her use since last semester. Both are very talented musicians, and they are my music friends.

Alan was a remarkable human being. I am so proud of him, and also his discovery by continuing inspiring the young generation regardless of the scientific field. He loved meeting new people from various fields and age groups all his life. I am sure he would feel very lucky to be admired by countless people.

I, once again, express my heartfelt gratitude to you all for gathering to celebrate his 100<sup>th</sup> birth anniversary.





https://schoengeometry.com/tmp/alansmathmind.mp4 https://photos.app.goo.gl/KtXzQ3WDHSu5mCY89

#### Gyroid Jingle (Anon.)

Fritz Laves found a crystal net with edges joined by threes, It twists and turns throughout R3 in perfect helices. This net has two varieties – to left or right they spiral. When two are intertwined the combination isn't chiral.

'Twixt two such nets a curving surface wends its way through space, With tunnels everywhere that make it look just like old lace. Now some do say the cosmos uses pasta<sup>1</sup> as its model. (If that's too big a stretch for you, you could just say it's twaddle.)

R. Wagner wrote some famous operas, staging them at Bayreuth, A place with several rhyming words – there's thyroid and there's gyroid, And that's the name by which we know this anticlastic surface, Whose labyrinths are such a maze they're bound to make you nervous.

We hear that gyroid shapes are formed in heav'n in some stars. (There's no report that this occurs on Venus or on Mars.) Such stars are not the common types like Capricorn or Castor, But rather they're like neutron stars (which spin around much faster).

Since many words do rhyme with 'G', like brie and ghee and plea, To simplify this verse we'll call the gyroid simply G. Schwarz, Weierstrass, and Riemann taught us long ago to see That G's the offspring of two others known as P and D.

There's Single G and Double G. Which one do you like more? Since both occur in Nature, there's no point in keeping score. <sup>2</sup>Luzzati found that Double G can crystallize as soap, And in the soap domain he's known world over as the Pope.

Cosmologists say the universe arose by chance – not purpose. So we conclude the gyroid's just an accidental surface. Vittorio<sup>2</sup> found its structure hidden in a plain detergent. And now phenomena like this are properly called emergent.

<sup>1</sup>Appearance of the Single Gyroid Network Phase in Nuclear Pasta Matter, arXiv:1404.4760v5 [nucl-th] 31 Oct 2014, B. Schuetrumpf, M. A. Klatt, K. Iida, G. E. Schroeder-Turk, J. A. Maruhn, K. Mecke, P.-G. Reinhard

<sup>2</sup>Luzzati, V. and Spegt, P. A., Nature, **215**, 701 (1967)

#### Gyroid Jingle (Anon.)

Fritz *La*-ves *found* a *crys*-tal *net* with *ed*-ges *joined* by *threes*, It *twists* and *turns* through-*out* R-3 in *per*-fect *he*-li-*ces*. This *net* has *two* var-*i*-*e*-*ties* – to *left* or *right* they *spi*-ral. When *two* are *in*-ter-*twined* the *com*-bi-*na*-tion *is*-n't *chi*-ral.

'Twixt *two* such *nets* a *curv*-ing *sur*-face *wends* its *way* through *space*, With *tun*-nels *ev*-ery-*where* that *make* it *look* just *like* old *lace*. Now *some* do *say* the *cos*-mos *u*-ses *pas*-ta<sup>1</sup> *as* its *mod*-el. (If *that's* too *big* a *stretch* for *you*, you *could* just *say* it's *twad*-dle.)

R. *Wag*-ner *wrote* some *fa*-mous *op*-eras, *sta*-ging *them* at *Bay*-reuth, A *place* with *seve*-ral *rhym*-ing *words* – there's *thy*-roid *and* there's *gy*-roid, And *that's* the *name* by *which* we *know* this *an*-ti-*clas*-tic *sur*-face, Whose *lab*-y-*rinths* are *such* a *maze* they're *bound* to *make* you *ner*-vous.

We *hear* that *gy*-roid *shapes* are *formed* in *heav*-'n *in* some *stars*. (There's *no* re-*port* that *this* oc-*curs* on *Ve*-nus *or* on *Mars*.) Such *stars* are *not* the *com*-mon *types* like *Cap*-ri-*corn* or *Cas*-tor, But *rath*-er *they're* like *neu*-tron *stars* (which *spin* a-*round* much *fast*-er).

Since *man*-y *words* do *rhyme* with 'G', like *brie* and *ghee* and *plea*, To *sim*-pli-*fy* this *verse* we'll *call* the *gy*-roid *sim*-ply G. Schwarz, *Wei*-er-*strass*, and *Rie*-mann *taught* us *long* a-*go* to *see* That G's the *off*-spring *of* two *oth*-ers *known* as *P* and *D*.

There's *Sing*-le *G* and *Doub*-le *G*. Which *one* do *you* like *more*? Since *both* oc-*cur* in *Na*-ture, *there's* no *point* in *keep*-ing *score*. <sup>2</sup>Luz-*za*-ti *found* that *Doub*-le *G* can *crys*-tal-*lize* as *soap*, And *in* the *soap* do-*main* he's *known* world *o*-ver *as* the *Pope*.

Cos-molo-gists say the u-ni-verse a-rose by chance – not pur-pose. Well, that im-plies the gy-roid's just an ac-ci-dent-al sur-face. Vit-tori-o<sup>2</sup> found its struct-ure hid-den in a plain de-ter-gent. And now phe-nom-e-na like this are proper-ly called e-mer-gent.

<sup>1</sup>Appearance of the Single Gyroid Network Phase in Nuclear Pasta Matter, arXiv:1404.4760v5 [nucl-th] 31 Oct 2014, B. Schuetrumpf, M. A. Klatt, K. Iida, G. E. Schroeder-Turk, J. A. Maruhn, K. Mecke, P.-G. Reinhard

<sup>2</sup>Luzzati, V. and Spegt, P. A., Nature, **215**, 701 (1967)

## **General Information**

## Welcome Reception

Welcome reception will be held in BLOSSOM CAFÉ 3F (See the Map) from 18:00 on November 19.

## Lunch

Those who applied lunch boxes will receive "**Exchange Ticket**" at registration desk. You will take a lunch box at BLOSSOM CAFÉ 3F (See the Map) using the ticket.

## Excursion

It will be held on November 21. We will depart at 12:20 and go Sumiyoshi Taisha Shrine, Yamamoto Noh Theater, Osaka Castle. Please check the shuttle bus departure point on the map in the next page.



## **Conference** Dinner

It will be held on November 21 at Osaka Geihinkan from 17:30 to 19:30.

## Session Format

#### **Oral Session**

Oral session will be held at November Hall (See the Map). For the sake of lively discussion, please strictly respect the following maximal talk times allocated for your presentations,

Tutorial Lecture: 55 min (45 min presentation + 10 min questions) Plenary Lecture: 40 min (35min presentation + 5 min questions) Invited Lecture: 30 min (25 min presentation + 5 min questions) Contributed Lecture: 20 min (15 min presentation + 5 min questions)

#### **Poster Session**

#### November Hall

- Poster session will be held at BLOSSOM CAFÉ 3F (See the Map).
- Please post at the first day, and remove the poster at the lunch time on the final day.
- Presentation time is from 15:20 to 17:20 on November 20.
- Those with odd numbers should present in the first half (15:20 to 16:20), and those with even numbers should present in the second half (16:20 to 17:20).

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#### Lecture Hall

November Hall



#### **Poster & Lunch**

BLOSSOM CAFÉ 3F



## Shuttle Bus (Tennoji-Kindai, Kindai-Tennoji)

Nov. 19 (Tue.): Morning 8:40-9:20, Return 19:15-19:55

Nov. 20 (Wed.): Morning 8:00-8:40, Return 17:30-18:10

Nov. 21 (Thu.): Morning 8:00-8:40, Excursion

Nov. 22 (Fri.): Morning 8:00-8:40, Return 14:30-15:10



## WiFi information

Participants can access WiFi in November Hall, Blossom Cafe, Academic Theater (Biblio Theater) with the SSID and PW as below.

SSID: GyroidIsEverywhere-WiFi

PW: Schoen-100th-Birth

#### Alan Schoen 100th birth anniversary

#### Gyroid is everywhere

Date November 19 - 22, 2024

Venue: November Hall, Kindai University, HigashiOsaka, Japan

#### Program

#### November 19 (Tue)

9:00 - 9:50	Registration
9:50 - 10:00	Tomonari Dotera (Kindai University)
	Welcome remark, Introduction of Alan Schoen
10:00 - 10:10	Itaru Matsumura (President, Kindai University)
	Opening address

#### Chair: Tomonari Dotera

# Tutorial lectures (Open lectures w/o registration)10:10 - 11:05Randall Kamien (University of Pennsylvania)<br/>Materials Geometry11:05 - 12:00Stephen Hyde (Sydney University & Australian National University)<br/>Triply periodic minimal surfaces revisited: surface complexes

12:00 - 13:30 Lunch (BLOSSOM CAFÉ 3F)

#### Chair: Gerd Schröder-Turk

#### **Plenary lecture**

13:30 - 14:10Myfanwy Evans (University of Potsdam)Gyroid as an organiser of entanglement

#### **Invited lectures**

14:10 - 14:40	Jacob Kirkensgaard (University of Copenhagen)
	Exploring pattern formation on negatively curved surfaces via the hyperbolic
	plane
14:40 - 15:10	Koya Shimokawa (Ochanomizu University)
	Polycontinuous pattern and 3-dimensional topology

15:10 - 15:40 **Coffee break** 

#### Chair: Randall Kamien

#### **Contributed presentations**

15:40 - 16:00	Hao Chen (ShanghaiTech University)
	Recent mathematical progress on Triply Periodic Minimal Surfaces, and how
	physics inspired them
16:00 - 16:20	Chern Chuang (University of Nevada, Las Vegas)
	Square lattice representations of P, D, and G surfaces and their mixtures and
	generalizations
16:20 - 16:40	Kanata Warisaya (The University of Tokyo)
	Reconfigurable Periodic Surfaces Assembled from Strip Modules

16:40 - 16:50 Break

#### Chair: Stephen Hyde

#### **Contributed presentations**

16:50 - 17:10	Toshihiko Oka (Shizuoka University)
	Investigating electron density of gyroid structures by X - ray diffraction
17:10 - 17:30	Goran Ungar (Xi'an Jiaotong University)
	Skeletal bicontinuous mesophases of bundled axial rod-like molecules
17:30 - 17:50	Osamu Terasaki (ShanghaiTech University)
	Where and how we have met and learnt from G-surface

17:50 - 18:00	Move
18:00 - 19:00	Welcome reception (BLOSSOM CAFÉ 3F)
	Reiko Schoen (Mrs. Schoen)
	Yushu Matsushita (Toyota Physical and Chemical Research Institute)
	Greeting & Toast

#### November 20 (Wed)

#### Chair: Yushu Matsushita

#### **Plenary lecture**

9:00 - 9:40	Ulrich Wiesner (Cornell University)
	Co-Continuous Gyroidal Hybrid Nanomaterials from Block Copolymer
	Self-Assembly

#### **Invited lectures**

9:40 - 10:10	Rong-Ming Ho (National Tsing Hua University)
	Network Phases from Self-Assembly of High Interaction Parameter Block
	Copolymers and Chiral Block Copolymers
10:10 - 10:40	An-Chang Shi (McMaster University)
	Stabilizing network phases of block copolymers

#### 10:40 - 11:10 **Coffee break**

#### Chair: Osamu Terasaki

#### **Contributed presentations**

11:10 - 11:30	<b>Lu Han</b> (Tongji University)
	Formation of Triply Periodic Hyperbolic Surface Structures via Block
	Copolymer Self-Assembly
11:30 - 11:50	<b>Weihua Li</b> (Fudan University)
	Stabilize different continuous network phases by rationally designing block
	copolymers
11:50 - 12:10	Atsushi Takano (Nagoya University)
	Novel Tricontinuous Microphase-Separated Structures formed from ABC
	Triblock Terpolymer Blends

12:10 - 13:30 Lunch (BLOSSOM CAFÉ 3F)

#### Chair: Goran Ungar

#### **Invited lectures**

13:30 - 14:00	Xiangbing Zeng (University of Sheffield)
	How Do You Make a Gyroid Chiral?
14:00 - 14:30	Takahiro Ichikawa (Tokyo University of Agriculture and Technology)
	Gyroid Minimal Surface as Proton Conduction Pathway

#### **Contributed presentation**

14:30 - 14:50 Shoichi Kutsumizu (Gifu University)

Control of  $Ia\overline{3}d$  Gyroid phase formation in aryloyl-hydrazine-based molecules by using two chemical modifications, introducing the side group and slight non-symmetry into the core moiety

14:50 - 15:20 **Coffee break** 

#### 15:20-17:20 **Poster Session**

Poster size: A0 (board width 900 mm) You can display your poster from November 19 to 22.

#### November 21 (Thur)

#### Chair: Jacob Kirkensgaard

#### **Plenary lecture**

9:00 - 9:40Gregory Grason (University of Massachusetts Amherst)Fitting into and shifting symmetries of block copolymer cubic networks

#### **Invited lectures**

9:40 - 10:10	Philipp Schönhöfer (University of Michigan)
	"Challenging" Steiner's formula: Pathways to stabilize the gyroid in colloidal
	self-assembly
10:10 - 10:40	Justin Llandro (Sumitomo Chemical Co., Ltd.)
	Magnetism and topology in self-assembled 3D gyroid nanostructures

#### 10:40 - 11:10 **Coffee break**

#### Chair: Kunio Awaga

#### **Contributed presentations**

11:10 - 11:30	Jun-ichi FUKUDA (Kyushu University)
	Structural transformation of cholesteric blue phases revealed by continuum
	simulation and machine-learning-aided structural analysis
11:30 - 11:50	Masahisa Tsuchiizu (Nara Women's University)
	Topological electronic states in microscopic gyroids
11:50 - 12:10	Rie Suizu (Nagoya University)
	Coexistence of Collinear and Non-collinear Spin Texture in Antiferromagnetic
	Gyroidal MOFs

#### 12:10 - **Excursion**

Lunchbox Sumiyoshi Taisha Shrine Yamamoto Noh Theater Osaka Castle

Dinner (OSAKA GEIHINKAN) Randall Kamien (University of Pennsylvania) Toast

#### November 22 (Fri)

#### Chair: Myfanwy Evans

#### **Plenary lecture**

9:00 - 9:40 Matthias Saba (University of Fribourg) *Gyroid Photonics – From Chiral Beamsplitters and Active Materials to Topological Physics and Bound States in the Continuum* 

#### **Invited lectures**

9:40 - 10:10	Vinod Kumar Saranathan (University of Tours)
	Functional Morphology of Mesoscale Organismal Single Gyroids
10:10 - 10:40	Łucja Kowalewska (University of Warsaw)
	Beyond the Ordinary: Diamond- and Gyroid-Shaped Membranes in Plant
	Plastids

10:40 - 11:10 **Coffee break** 

#### Chair: Matthias Saba

#### **Contributed presentations**

11:10 - 11:30	Annie Jessop (Murdoch University)
	Reflections from a developing butterfly Gyroid
11:30 - 11:50	Shigeru Okamoto (Nagoya Institute of Technology)
	A Single Grain of OBDG in a Semi-dilute Solution - Photonic Crystal

11:50 - 12:50 **Lunch** (BLOSSOM CAFÉ 3F)

#### Chair: Takahiro Ichikawa

#### Invited lecture

12:50 - 13:20	<b>Kunio Awaga</b> (Nagoya University)
	Rational Synthesis of Molecular Gyroids and their Structure-Derived
	Solid-State Properties

#### **Discussion & Summary**

13:20 - 14:00 Gerd Schröder-Turk (Murdoch University)

#### **Closing remark**

14:00 - 14:10 **Stephen Hyde** (Sydney University & Australian National University)

November 20 (Wed)15:20-17Poster SessionPoster si

15:20-17:20 *Poster size: A0 (board width 900 mm)* 

#### **Mathematics**

1-1	Toky Andriamanalina (University of Potsdam)
	Unknotting 3-periodic entanglements of filaments and nets
1-2	Martha Dunham (Independent Researcher)
	Macro Scale Gyroid Applications
1-3	Hou-Hsun Ho (National Taiwan University)
	Discrete Gyroid Structures: Defect-Driven Tiling and Analogies with Zeolite
	Frameworks
1-4	Sonia Mahmoudi (Tohoku University)
	Construction and Classification of Hyperbolic Diagrams and their Triply Periodic
	Weavings & Polycatenanes via Mapping to the Gyroid
1-5	Yukihiro Nishikawa (Kyoto Institute of Technology)

*Curvature Estimation based on Distance Conversion of a 3D image* 

#### **Physics**

2-1	Greg Grason (University of Massachusetts Amherst)	
	Design economy and assembly of size-programmable triply-periodic polyhedra from	
	addressable nanotriangles	
2-2	Matthias Himmelmann (University of Potsdam)	
	Exploring the Homogeneity of Disordered Minimal Surfaces	
2-3	Suman Kulkarni (University of Pennsylvania)	
	On characterizing the topology and geometry of imperfect gyroids.	
2-4	Vira Raichenko (University of Potsdam)	
	Cocoon Microstructures through the Lens of Topological Persistence	
2-5	Hideaki Tanaka (Sango Co., Ltd.)	
	Programmable Self-Assembly of Nanoplates into Bicontinuous Nanostructures	
2-6	Kana Yamamoto (Kindai University)	
	Hexagulation numbers: magic numbers on the gyroid surfaces	
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## Chemistry

Noriyoshi Arai (Keio University)
Molecular understanding of mechanical properties of Archimedean tiling through star
terpolymer thin film

- **3-2** Yifei Cheng (Fudan University) Understand the Relative Stability of Single-Gyroid to Double-Gyroid in AB-type Block Copolymer
- **3-3 Qingshu Dong** (Fudan University) *Hybrid Structures Formed by Asymmetric ABC-type Block Copolymers*

- 3-4 Takashi Honda (Ochanomizu University) Molecular Weight Dependence of Domain Spacing in the Double Gyroid Structure of ABC Triblock Copolymers 3-5 **Shuto Ito** (Biomatter Lab) Polymer Membrane Tensegrity: Inverse Design of Polymer Films Morphing into Arbitrary 3D Surfaces with Digital Photopatterning Technique 3-6 Shinichi Sakurai (Kyoto Institute of Technology) Changes in two-dimensional small-angle X-ray scattering pattern by uniaxial stretching of a double-gyroid block copolymer 3-7 **Qingliang Song** (Fudan University) Hierarchical Self-assembly Behaviors of ABC-Type Bottlebrush Copolymers 3-8 **Jiro Suzuki** (High Energy Accelerator Research Organization (KEK)) Gyroid Interface from Symmetric ABCD Tetrablock Quarterpolymers by Monte Carlo Simulation 3-9 Naoya Torikai (Mie University) Interfacial Segment Distribution of a Diblock Copolymer in a Polymer Thin Film 3-10 Xintong You (Fudan University) Hierarchical gyroid structures in frustrated ABC triblock copolymers 3-11 **Xiangbing Zeng** (University of Sheffield)
  - Stage-wise Pre-assembly in Melt Prior to Liquid Crystals

#### Biology

- **4-1 Chisaki Kitajima** (Kyushu University) Structures made by termites and spiders
- **4-2** Allan Millsteed (Murdoch University) Order and disorder of the microstructures of the Cidaris rugosa sea urchin stereom
- 4-3Ryosuke Ohnuki (Tokyo University of Science)Chirality of gyroid-type photonic crystals in the scale of Teinopalpus Imeperialis

#### Engineering

- 5-1 Abdulaziz Alsenafi (Kuwait University) Non-Fourier Computations of Heat and Mass Transport in Nanoscale Solid-Fluid Interactions Using the Galerkin Finite Element Method
  5-2 Ziad Saghir (Toronto Metropolitan University)
- Heat enhancement using Gyroid Structure and metal foam for Different Porosity and Cooling fluids: Experimental and Numerical Approaches
- 5-3 Kaixin Yan (Beihang University) Coupling Additive Manufacturing with Triply Periodic Minimal Surface Enable Next-Generation Aero-Engine Heat Exchangers
- 5-4Takumi Yano (Kindai University)Sound Insulation Properties of Gyroids at Normal Incidence



Alan Schoen 100th birth anniversary Gyroid is everywhere November Hall, Kindai, Osaka, Japan Tutorial Lectures Nov. 19 (2024)

#### <u>Randall Kamien</u>

Professor Randall Kamien is the Vicki and William Abrams Professor in the Natural Sciences and a professor of physics and astronomy in the Department of Physics and Astronomy at the University of Pennsylvania. He also holds a secondary appointment in mathematics. Kamien is a leading figure in the theory of topological effects in soft condensed matter physics, renowned for the mathematical rigor he brings to his work. Particularly, he is



recognized for his use of sophisticated and elegant geometrical methods to gain insight into fundamental aspects of the structure of polymers, colloids, liquid crystals, and related materials, as well as into the topological defects occurring in these materials. His strong reputation and broad knowledge across many areas of physics are further evidenced by his roles as Lead Editor of the Journal of Modern Physics since 2017 and APS Editor in Chief (including the Physical Review series) since the beginning of 2023. Kamien has been a Simons Investigator and has received numerous awards, including the G.W. Gray Medal and the Samsung Mid-Career Award. Additionally, he has received fellowships from the American Association for the Advancement of Science, the American Physical Society, and the Alfred P. Sloan Foundation. He earned his Ph.D. from Harvard University in 1992. Prof. Kamien is also well-known for delivering high-quality and enthusiastic lectures.

#### Stephen T. Hyde

Professor Stephen Timothy Hyde is an Australian scientist who was appointed a Fellow of the Australian Academy of Science in 2005. He is a professor and also the ARC Federation Fellow in the Department of Applied Mathematics, Research School of Physics, at the Australian National University. In 2021, he took up a position at the University of Sydney. His specialty is in the field of theoretical



physics, focusing on the self-assembly of complex materials and systems. He is interested in the structuring of complex physical, geological, and biological systems and the relevance of lowdimensional geometry and topology. Physical structures include the self-assembly of molecular and macromolecular amphiphiles and lipids in solution into liquid crystals, as well as the formation of inorganic materials in biological and abiotic conditions. Novel hyperbolic interfaces and bicontinuous spatial partitions, including the gyroid, are of particular interest to him. He also works on the characterization and enumeration of geometric networks in various spaces, including two-dimensional hyperbolic networks and higher-dimensional Euclidean networks, using techniques from graph theory and topology. He is one of the authors of "*The Language of Shapes, The Role of Curvature in Condensed Matter: Physics, Chemistry and Biology*," which is the most famous books in the field.



Alan Schoen 100th birth anniversary Gyroid is everywhere November Hall, Kindai, Osaka, Japan Tutorial Lectures Nov. 19 (2024)

#### <u>ランドール・カミエン教授</u>

ランドール・カミエン教授は、ペンシルベニア大学の物理天 文学学科の物理学教授であり、ビッキー&ウィリアム・エイ ブラムズ職自然科学教授でもあります。同時に数学科の教授 でもあります。カミエン教授は、ソフトマター凝縮系物理学 のトポロジカル効果の理論で著名な研究者であり、数学的厳 密さで知られています。特に、彼は洗練された簡明な幾何学



的手法を使用して、高分子、コロイド、液晶などの物質構造の原理的側面とこれらの物質 に発生するトポロジカル欠陥に対する鋭い洞察力で知られています。彼への評価の高さと 物理学の多くの分野にわたる広範な知識は、2017 年以来「Journal of Modern Physics」 の編集長としての役割や、2023 年初めからのアメリカ物理学会(Physical Review シリー ズの)総編集長としての役割でも明らかです。カミエン教授はサイモンズ研究者であり、 G.W. グレイメダルやサムスンミッドキャリアアワードなど、数々の賞を受賞しています。 さらに、アメリカ科学振興協会、アメリカ物理学会、アルフレッド P. スローン財団から奨 学金を受けています。彼は 1992 年にハーバード大学で博士号を取得しました。カミエン 教授は情熱あふれる名講義を行うことでも有名です。

#### <u>スティーブン・ハイド教授</u>

スティーブン・ティモシー・ハイド教授は、2005年にオー ストラリア科学アカデミーのフェローに任命されたオース トラリアの科学者で、オーストラリア国立大学の物理学部 門応用数学科の教授であり、またオーストラリア研究評議 会 (ARC)連邦特別研究員でもあります。2021年にはシド ニー大学化学部門でポジションを得ました。彼の専門は理



論物理学の分野で、複雑な物質や系の自己組織化に焦点を当てています。彼は複雑な物理 系、地質系、生命系での構造化と低次元幾何学及びトポロジーの関連性に興味を持ってい ます。研究対象となる物質構造として、溶液中の分子および高分子からなる両親媒性物 質、リン脂質液晶系、それらの自己組織化や、生物学的および非生物学的条件下での無機 材料の構造形成などが含まれます。ジャイロイドや新しい双曲面の界面による共連続構造

(空間分割)が特に関心の中心です。彼はまた、グラフ理論とトポロジーの手法を用い て、2次元の双曲的ネットワークや高次元のユークリッド空間の幾何学的ネットワークの 分類と数え上げにも取り組んでいます。彼はこの分野で最も有名な書籍「形の言語、凝縮 物質における曲率の役割:物理学、化学、生物学」の著者の1人です。 Tutorial lectures 10:10 - 11:00, November 19 (Tue)

#### **Materials Geometry**

#### Randall D. Kamien\*

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Why is geometry so effective as a tool in the study of materials? Why do physical systems extremize energies? Calculus of variations is such an essential part of our formulation of the world and geodesics are the fundament of geometry. I will give a few examples where the power of geometric logic provides an express route to the understanding of complex These will include the systems. knitting shown on the right, analysis of diblock copolymers, and the packing of There will be soft spheres. demonstrations.

This work was supported by the Simons Foundation and pure thought.



#### **Triply periodic minimal surfaces revisited: surface complexes**

Stephen T. Hyde<sup>1,2,\*</sup>, Liliana de Campo<sup>3,^</sup> and Alan H. Schoen<sup>†</sup>

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Alan Schoen made many contributions to physics and geometry beyond the Gyroid, some of which have been described in a recent obituary (ref. 1). The Gyroid, like Schwarz' P and D triply-periodic minimal surfaces (TPMS), define a pair of catenated 3d labyrinths and are *bicontinuous*. These surfaces partition 3d euclidean space into *two* extended three-periodic open cells, bounded by the TPMS. In that sense they generalise simpler classical space partitions, namely the tessellation of 3d euclidean space by an *infinite* number of plane-faced polyhedra, e.g. congruent cubes or "saddle polyhedra" - whose faces are curved minimal surfaces - explored by the architect Paul Pearce (ref. 2).

Both labyrinths of TPMS were perceived by Schoen as inflated three-periodic skeletal nets (or "labyrinth graphs"). By analogy saddle polyhedral cells, which are topological balls, are zero-periodic. These examples of cellular decompositions of space suggest more general lines of inquiry. If we constrain the cells to be bounded by faces which are minimal surfaces:

- (i) can we find partitions of of 3d euclidean space beyond zero- and three-periodic cases?
- (ii) can space be partitioned into z equal cells, apart from z=2 (TPMS) or  $z=\infty$  (polyhedral tessellations)?

The answers are yes and yes. Simpler cases are self-intersecting TPMS, many of which Schoen explored (in ref. 3), succeeded by the crystallographic studies of Fischer and Koch (e.g. refs. 4, 5). Later on, we found a number of three-periodic minimal *surface complexes (TPMS\*)*, which include three-fold branched lines (e.g. ref. 6) which include novel *polycontinuous* partitions for molecular self-assemblies (ref. 7).

In fact, Schoen had explored TPMS\* earlier, which he called "integral varifolds" (ref. 3). On meeting Schoen in 2011, all three authors of this paper decided to revisit his earlier study. We have reanalysed a complete suite of minimal surface Flächenstücke bounded by skew quadrilaterals which coincide with two-, three (and four-) fold axes of rotational symmetry of the cube. Among many more cases, twelve TPMS\* with cubic symmetry emerge, containing zero-, one-, two- and three-periodic cells, afford a rich inventory of partitions satisfying both (i) and (ii) above. Interesting examples - some of which have been derived independently by Longdell, Oguey and Hyde (unpublished) - include TPMS\* whose skeletal nets describe well-known crystallographic rod-packings and novel mutually catenated inclined meshes. A tetracontinuous TPMS\* contains a quartet of like-handed *srs* skeletal nets (in contrast to the enantiomeric pair of srs nets characterising the Gyroid). The most spectacular TPMS\* defies all intuition: it partitions 3d space in to a *single* three-periodic cell!

[1] Stephen T Hyde and Gerd E Schroeder-Turk (2024) Physics Today.

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- [6] Hyde, Stephen T., Liliana de Campo, and Christophe Oguey. (2009) Soft Matter 5(14), 2782-2794.
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Plenary lecture 13:30 - 14:10, November 19 (Tue)

#### Gyroid as an organiser of entanglement.

<u>Myfanwy E. Evans</u><sup>1,\*</sup>, Stephen T. Hyde<sup>2,3</sup> <sup>1</sup>University of Potsdam, Institute for Mathematics, Potsdam, Germany <sup>2</sup>Australian National University, Canberra, Australia <sup>3</sup>University of Sydney, Sydney, Australia \*email: evans@uni-potsdam.de

Three-dimensional structures can be complicated to describe. This talk introduces the use of the gyroid as a scaffold for constructing entanglement, utilising its elegant geometry to organise structures in a way that we can describe. Such entanglements are seen in polymer simulations [1], but the use of the gyroid, and the related srs net, also allows for extensive descriptions of complicated entanglement through simple combinatorial encodings.



[1] J. J. K. Kirkensgaard, M. E. Evans, L. de Campo and S. T. Hyde, PNAS, 111, 1271-1276 (2014).

## Exploring pattern formation on negatively curved surfaces via the hyperbolic plane

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We investigate the self-assembly behaviour of block copolymers constrained to thin hyperbolic films. Specifically, we study the pattern formation on the three-periodic cubic minimal surfaces P, D and G found ubiquitously in soft matter material science. We use a new method for visualisation and analysis of the patterns by mapping to two-dimensional hyperbolic space analogous to stereographic projections in cartography thus effectively creating a more accessible "hyperbolic map" of the pattern [1]. This allows us to pinpoint in detail the role of intrinsic geometry and to probe the role of negative curvature on the resulting assemblies as contrasted with flat and positively curved films. We present results from AB diblock copolymers and ABC mikto-arm star terpolymers of varying composition. In the case of compositionally balanced diblocks, the resulting patterns are related to ``free" tilings of the hyperbolic plane [2,3] while unbalanced molecules form a plethora of disc packings. Star polymers form three-colored cellular patterns related to curved graphene-like schwarzites constrained to only form even polygons.

Keywords: block copolymers, self-assembly, triply periodic minimal surfaces, hyperbolic geometry.



Figure 1. AB diblock copolymers self-assembling on the P-surface and mapped to the hyperbolic plane for analysis [1].

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#### Polycontinuous pattern and 3-dimensional topology

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In this talk, we explore the concept of handlebody decomposition of 3-manifolds, extending beyond the well-known Heegaard splittings and trisections. A handlebody decomposition divides a closed orientable 3-manifold into several handlebodies. Our main result demonstrates that two handlebody decompositions of a closed orientable 3-manifold are stably equivalent, meaning they become isotopic after a finite number of stabilizations. This generalization provides a new perspective on the structural properties of 3-manifolds.

We apply this theoretical framework to materials science by modeling polycontinuous patterns, which arise in the microphase separation of block copolymer melts. These patterns can be viewed as triply periodic non-compact surfaces, tribranched surfaces, or polyhedra embedded in R<sup>3</sup>, dividing it into

multiple submanifolds. Our model characterizes bicontinuous, tricontinuous, and polycontinuous patterns, which are of significant interest for understanding the morphology of copolymer systems.

A key aspect of our study is the correspondence between triply periodic polycontinuous patterns and handlebody decompositions of the 3-dimensional torus  $T^3$ . We show that such patterns, under suitable conditions, induce handlebody decompositions of  $T^3$ . Consequently, the Reidemeister-Singer-type theorem for handlebody decompositions extends to polycontinuous patterns, offering insights into their structural equivalence and transformation.



Through this topological approach, we provide a mathematical foundation for the classification and analysis of complex copolymer structures, highlighting the interplay

Figure 1 Nets and tricontinuous pattern.

between 3-manifold topology and material science. Our results not only advance the theoretical understanding of 3-manifolds but also have practical implications for designing novel materials with desired mechanical properties.

This work was supported by MEXT Grants-in-Aid for Scientific Research on Innovative Areas (JP17H06460 and JP17H06463) and JSPS KAKENHI grant no. JP21H00978.

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## Recent mathematical progress on Triply Periodic Minimal Surfaces, and how physics inspired them

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New Triply Periodic Minimal Surfaces (TPMSs) of genus 3 have been recently discovered. Some were explicitly constructed, others implicitly. I will review the mathematical techniques, in particular those involved in the existence proof of the deformations of the Gyroid. The new techniques will lead to even more new TPMSs of genus 3, which we are numerically aware of and determined to work on in the near future. Interestingly, all these mathematical results were heavily inspired by soft-matter physics. So I will also tell the stories of this interdisciplinary collaborations.

Some of the works to be presented was supported by Individual Research Grant from Deutsche Forschungsgemeinschaft within the project \Defects in Triply Periodic Minimal Surfaces", Projektnummer 398759432. Collaborators include Martin Traizet, Matthias Weber, Daniel Freese, etc.

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- [6] Chen, Hao; Freese, Daniel. Proc. A. 478 (2022), no. 2267, Paper No. 20220431, 18 pp.

## Square lattice representations of P, D, and G surfaces and their mixtures and generalizations

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We present a constructive mechanism for the P, D, and G triply periodic minimal surfaces and their hybrids by utilizing a decomposition reflecting the tetragonal lattice symmetry. In this context, the surfaces can be seen as filling in a square lattice with infinitely long 1D strips (with tetragonal boundary condition), where P strips are disjoined catenoids vertically stacked, D strips twisted helicoids, and G strips somewhere in between. This is reminiscent of the catenoid-helicoid transformation and/or the Bonnet transformation. Except for the P surface, both G and D strips trace out a helical boundary curves on the surface of the tetragonal cell and are chiral. By assuming glide symmetry planes along the grids of the square lattices, one recovers the original Schwarz P, D and Schoen's G surfaces. See Figure 1.

It becomes rather clear that such decomposition allows one to mix D and G strips together and form a hybrid D/G surface. It is unclear that such topology allows a minimal surface. However, since they share the same tetragonal boundary condition, one can create a seamless transition between a purely D compartment and a purely G one, essentially forming а grain boundary between the two semi-infinite surfaces. The 2D unit cell can be arbitrarily large with arbitrarily large genus.

By adjusting the boundary curve of P strips, referred to as a P' strip, one can also seamlessly join them with D or G ones and form hybrid surfaces/grain boundaries. A 3D cubic lattice generalization is possible but will be left for future exploration.

This work was supported by the research startup funding from the University of Nevada, Las Vegas.



**Figure 1** (Top left) The P, G, and D strips. (Top right) Square lattices filled with single type strips with glide plane symmetry. (Bottom left) The P', G, and D strips. (Bottom right) Mix-matched square lattices giving rise to hybrid surfaces. The barred characters refer to glide-symmetric (reflected in the xz/yz plane and translated half a spacing in the z direction.) Here we utilize a graphitic structure representation where each vertex (sp2 carbon atom) is connected to three nearest neighbors.

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#### **Reconfigurable Periodic Surfaces Assembled from Strip Modules**

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Cellular structures composed of a shell of periodic surfaces have been attracting attention for their properties such as high stiffness for low density and partitioning space into two subvolumes. Since they have negative Gaussian curvature, they cannot be constructed by simply bending sheet material. This study aims to efficiently construct periodic surfaces from sheet material by assembling a single type of developable pieces. The existing method [1] allows dividing some of the triply periodic minimal surfaces (P, D, and G surfaces) into a single type of narrow strip by periodic geodesic net connecting monkey saddles on them. We apply this division method to P, D, and G surfaces of constant negative Gaussian curvature, a family of surfaces with different slenderness (Figure 1), by assuming their existence. Due to the local isometry of the family, some elements of the family can consist of the congruent strip, enabling reconfiguration between surfaces with different topologies or slenderness (Figure 2). We fabricate physical models by approximating the strip with a developable surface (Figure 3). The straight strip allows for a high efficiency of material and can be cut from a roll of sheet. We believe this reconfigurable modular system can be a new geometric basis for self-build and self-assembly assuming disassembly and reconstruction.

This work was supported by JST AdCORP ``Realization of people- and environment-friendly artifacts by leveraging computational design and fabrication".

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Figure 1 Varying slenderness of G surface by transforming base grid on hyperbolic plane.



Figure 2 Reconfigurable pair of G surfaces with different slenderness and their flattened strip module.



Figure 3 Physical prototype. Both D and G surfaces are assembled from single type of strip module.

#### Investigating electron density of gyroid structures by X-ray diffraction

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To investigate the structure of nanoscale gyroid-like materials, it is essential to visualize the electron density. My collaborators and I have been developing a method to determine the electron density of gyroid phases of lyotropic liquid crystals by X-ray diffraction using monodomains (single-crystal regions). This method has enabled us to determine the electron density with unprecedented accuracy. Here, I will show the interface structure of the lyotropic liquid crystal gyroid phase revealed by the method. I also report the solution of the phase problem in the X-ray diffraction method.

In the gyroid phase of lyotropic liquid crystals, a microphase separation occurs between polar and nonpolar regions. The parallel surface (PS) model parallel to the gyroid surface and the constant mean curvature surface (CMCS) model were known as the interface structure. We investigated these interfacial structures for the gyroid phases of type I and type II lyotropic liquid crystals composed of amphiphilic molecules and water by single-crystal X-ray diffraction (ref. 1). For the observed X-ray diffraction data, we optimized the diffraction intensities expected from the two interface models. The PS model was clearly in better agreement with the observed data than the CMCS model. Judging from the degree of agreement, the interface is not in an intermediate state between the two models, but rather, it is much closer to the PS model. Figure 1 shows the electron density reconstructed from the amplitudes of the structure factors calculated from the observed intensity data and the phases calculated from the model. The high electron density (yellow) region of is the polar region, and a slightly lower density (orange) region locates near the center of the polar region. The electron density is slightly lower in the water-rich region within the polar region.

То determine the electron density from diffraction data, it is necessary to retrieve the lost phase information of the structure factor. This is called the phase problem. I have developed phase retrieval method а applicable to bicontinuous liquid crystal phases including gyroid phase (ref. 2). First, I found two indicators of the characteristics of bicontinuous liquid crystal phases that appear in the electron density. I found that electron



**Figure 1** Electron density of lyotropic liquid crystal gyroid phases. (Left) Type I, (Right) Type II. Yellow and blue are high and low electron density regions, respectively.

densities with small indicator vaclues tend to be the correct solution. I then developed an algorithm to find the correct electron density. Using these methods, the electron density of bicontinuous liquid crystal phases such as a gyroid phase can be easily obtained from diffraction data only. Using this method, we were also able to construct a new structural model of the chiral cubic phase of thermotropic liquid crystals (ref. 3).

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#### Skeletal bicontinuous mesophases of bundled axial rod-like molecules

Goran Ungar<sup>1,2,\*</sup>, Ya-xin Li<sup>3</sup>, Xiang-bing Zeng<sup>2,\*</sup>, Carsten Tschierske<sup>4</sup>, Feng Liu<sup>1</sup>

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There are 3 types of molecules forming bicontinuous mesophases (BM) in thermotropic liquid crystals: (a) end-chain-bearing rod-like and (b) fan-shaped molecules that lie in the network segments perpendicular to the segment axis, and (c) side-chain-bearing rod-like molecules which assemble in bundles that lie along segment axis. The fans (a) form exclusively double gyroid (DG), while rods (b) form DG and two other BMs not found in either lyotropics or block polymers: a triple-network cubic *I*23

and a double network tetragonal "Smectic-Q", both chiral. Because of packing problems, these compounds cannot form tetrahedral or octahedral junctions. However the axial bundle forming compounds (c) suffer no such restriction and have so far been found to form single diamond (SD), single primitive (SP), double network DG and DD, as well as alternating gyroid. Figure 1 explains how the size of the side-chains determines the type of phase. The schematic molecules in the figure are to scale with real molecules published in the numbered references: 28 [1], 30 [2], 31 [3], 32 [4]. SG and DP have not been found so far, as the required side-chains are, respectively, too long and too short. However we just found a way around the latter problem and obtained the first thermotropic DP, or "Plumber's nightmare" phase [5]. This will be described in the presentation.



volume in the unit cell that is closest to a given network segment and at a distance r from it. Inset is a view down the bundle. The time-averaged shape of the side-chain should closely match the space bounded by dV/dr and -dv/dr for a given phase.

*This work was supported by NSFC* (92156013, 92356306).

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#### Oral Presentation 17:30 - 17:50, November 19 (Tue)

#### Where and how we have met and learnt from G-surface

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To appreciate Alan Schoen's scientific impact to our community, we will focus on G-surface, among triply periodic minimal (TMP) G-, D- and P-surfaces, where three-dimensional (3d) silica-mesoporous -crystal (SMC) of MCM-48 with amorphous silica wall is formed.

Luzzati's group proposed structure of lipids; divalent polar groups were present on rods of finite length belonging to two interwoven infinite 3d-networks with *Ia-3d* space group symmetry and hydrocarbon chains constituted a continuous paraffin matrix. This corresponds to double gyroid [Nature 1967, **215**, 701], while a group of Mobil reported ordered mesoporous silica mesoporous crystals MCM-41 & MCM-48 (*Ia-3d*) from material aspects [Nature 1992, **359**, 710]. Discussions based on the quantum mechanics have been also reported indicating that the motion of electrons confined in curved geometry is different from that in 3D bulk crystals and relationship of electron energy bands among them [Ann. Phys. 1971, **63**, 586; PRA 1981, **23**, 1982; Prog. Theor. Phys. 1991,**106**, 235 & 1992, **88**, 229; PRB 2005, **72**, 085459].

We have developed a new electron crystallography (EC) to obtain unique structure solutions of 3d-SMCs, through an electrostatic potential distribution in real space, by Fourier analysis of a set of highresolution transmission-electron-microscope (HR-TEM) images, which has clearly indicated 3d-SMCs are formed through co-operative self-assembly of inorganic species with organic surfactants in water [J. Electron Microsc. 1999, **48**, 795; Nature 2000, **408**, 449.] Furthermore, a self-consistent structural solution of 3d-SMCs has been obtained from EC as a constant mean curvature (CMC) surface by minimizing the Helfrich energy density of the boundary between inorganic and organic mesophase components [Angew. Chem. Int. Ed. 2010, **49**, 8867]. This makes possible to follow structural changes from as synthesized to calcined state systematically. In addition, we wrote a chapter, "Electron crystallography" for crystallographic understandings on G-surface, double and single gyroids and their mutual relationship together with basic electron microscopy.

At the Conference, following "Electron crystallography" we will discuss crystallography and electron microscopy on G-surface, single and double gyroids, *i.e.*, diffraction patterns (X-ray & electrons), EM images, most-probable and unique structure solutions using our accumulated experimental data.

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#### Co-Continuous Gyroidal Hybrid Nanomaterials from Block Copolymer Self-Assembly

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#### ABSTRACT

Since the discovery of the Gyroid morphology in block copolymer self-assembly, this structure has fascinated polymer scientists around the world. This talk will discuss block copolymer self-assembly directed hybrid materials with double and single gyroid morphologies with a focus on the preparation of functional materials. To that end, diblock copolymers and triblock terpolymers will be used to structure direct inorganic components typically in the form of nanoparticles. Fundamental design criteria for successful periodic cubic gyroidal lattice formation of the resulting block copolymernanoparticle hybrids will be discussed. In addition to characterization of the as-made bulk hybrids, the talk will present the formation of mesoporous inorganic materials with gyroidal morphology from further thermal processing. It will be demonstrated how fundamental understanding of block copolymer co-assembly with inorganic nanoparticles allows these approaches to be generalized from meoporous amorphous oxides and high-temperature non-oxides to mesoporous highly crystalline transition metal oxides, metals, and seminconductors all the way to mesoporous superconductors. Associated applications range from separation technologies to energy conversion and storage all the way to catalysis. Special focus will be on the formation of block copolymer self-assembly directed mesoporous quantum metamaterials, where block copolymer mesostructure controls quantum materials properties beyond those of the intrinsic atomic lattice bulk structures.

#### Network Phases from Self-Assembly of High-χ Block Copolymers and Chiral Block Copolymers

#### **Rong-Ming Ho**

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Network Phases from the self-assembly of block copolymers (BCPs) have attracted extensive attention and intensive study over the years because of their appealing applications due to the effect of deliberate structuring on material properties inspired from nature.

By taking advantage of the effect of solvent selection on BCP self-assembly with tuning solvent evaporation rate for casting, a series of cubic network phases can be obtained from the self-assembly of single-composition, lamellae-forming polystyrene-*block*-polydimethylsiloxane (PS-*b*-PDMS) due to its high- $\chi$  character. An unusual network phase in diblock copolymers, double primitive phase (DP) (hexapod network) with space group of  $Im\bar{3}m$ , can be observed for the first time. With the reduction of solvent evaporation rate, double diamond phase (DD) (tetrapod network) with space group of  $(Pn\bar{3}m)$  and double gyroid (trigonal planar network) with space group of  $(Ia\bar{3}d)$  can be obtained due to the reduction on the degree of packing frustration (entropic penalty) within the junction (node).<sup>1</sup>

With the introduction of topology effect on PS-*b*-PDMS self-assembly, the phase window for network phase formation can be enlarged in self-assembled PS-*b*-PDMS. Apart from gyroid and diamond, a peculiar network phase with space group of Pm3n (Frank-Kasper structure) can be found for the first time as evidenced by small-angle X-ray scattering. Electron tomography results reveal the network phase with alternating connection of three and four struts. The observed phase behaviors suggest that the network formation is built from the bisectors of dispersive spheres in the Frank-Kasper phase, instead of building connections among them, and thus decipher the origins of complex phase formation due to the adaptive character of malleable mesoatoms.<sup>2</sup>

Block copolymers composed of chiral entities, denoted as chiral block copolymers (BCP\*s), were designed for mesochiral self-assembly. A helical phase was discovered for the first time in the self-assembly of BCPs. Homochiral evolution at different length scales in the self-assembly of the BCPs\* was found. Generalization of the chirality effect on the self-assembly of BCPs was established.<sup>3</sup> By extending the homochiral evolution concept of mesochiral self-assembly, it is feasible to fabricate nanonetwork phase with controlled helicity from self-assembly for the first time.<sup>4</sup>

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#### Stabilizing network phases of block copolymers

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Block copolymers are macromolecules composed of chemically distinct sub-chains or blocks connected via covalent bonds (**Figure 1**) [1]. The most distinguishing property of block copolymers is that they are intrinsically frustrated due to the inter-block repulsion and chain connectivity [2]. Alleviating the frustration leads to the formation of polymeric assemblies in the form of lamellae, cylinders and spheres. The packing of these soft objects results in a rich array of periodically ordered phases (**Figure 2**).

Among the ordered phases, the bicontinuous network phases, consisting of two interweaving networks composed of the minority-blocks embedded in a matrix of the majority blocks, are of particular interest due their intricate structures and potential applications. For linear AB diblock copolymers, extensive experimental and theoretical studies have established that the equilibrium network phase is dominated by the double-gyroids (**Figure 2**). On the other hand, there exists several bicontinuous structures, including the double gyroid ( $Ia\bar{3}d$ ), double diamond (Pn3m) and double-primitive ( $Im\bar{3}m$ ) phases. It is therefore desirable to explore the possibility to stabilize different network phases formed from block copolymers.

In order to the search for block copolymer systems that could stabilize different biconinuous structures, we have studied the relative stability of several network phases in binary blends of linear AB diblock copolymers and nonlinear miktoarm star copolymers by using the selfconsistent field theory (SCFT). For binary blends of AB diblock copolymers [3], our theoretical study predicts that the double-diamond and the double-primitive phases can be stabilized in binary blends composed of gyroid-forming and homopolymer-like diblock copolymers. Beyond linear architectures, our theoretical results indicate that a designed  $A'(A''B)_5$  miktoarm star copolymer can stabilize doublediamond and double-primitive network phases besides double-gyroid [4]. Mechanisms for stabilizing the networks are shown to be related to the relieving of the packing frustration and the regulation of the AB interfacial



Figure 1 Schematics of block copolymers.



**Figure 2** Phase diagram of conformationally asymmetric AB diblock copolymers obtained from SCFT.

curvature. These two mechanisms could act in tandem, resulting in larger stability regions for the novel network phases.

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# Formation of Triply Periodic Hyperbolic Surface Structures via Block Copolymer Self-Assembly

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Gyroid, diamond and primitive surfaces, the most famous naturally occurring triply periodic hyperbolic surfaces, are well known for their amazing properties closely associated with their intriguing symmetries. Basic research into the artificial synthesis and symmetry manipulations of these delicate structures is not only important for the preparation of novel functional materials, but also offers a general understanding of structure formation in soft matter and relevant biological systems.

Herein I will show the synthesis and symmetry manipulation of the hyperbolic surface structures based on the cooperative self-assembly of amphiphilic block copolymer soft template and the inorganic precursors. Particularly, I will discuss (i) A new tetragonal form of gyroid surface, termed Shifted tG, synthesized in a cooperative binary self-assembly system consisting of block copolymer and surfactant. (ii) The bottom-up approach to fabricate the single diamond surface titania networks using the diblock copolymer as a soft template and titania precursor, in which the single diamond scaffold was obtained by kinetically controlled nucleation and growth in the skeletal channels of the diamond minimal surface formed by the polymer matrix. (iii) The structural relationship and interconversion of different types of hyperbolic surface structures.



**Figure 1** Transmission electron microscopy images and reconstructed 3D volume of the tetragonal gyroid structure, featuring periodic distributions of uneven matrix thicknesses with a low-symmetry space group of  $I4_1/a$  (left). The cross-sectional backscattered scanning electron microscopy image, transmission electron microscopy image and the reconstructed 3D structure of the single diamond surface titania scaffold with space group of Fd-3m (right).

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# Stabilize different continuous network phases by rationally designing block copolymers

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The self-assembly of block copolymers provides an efficient method for the fabrication of ordered nanostructures. One of the most useful nanostructures is the bicontinuous network phase. For most of AB-type block copolymers, the stable network phase is the double-gyroid network structure, but not the other two network structures, i.e. double-diamond and double-primitive. It has been commonly accepted that the superior stability of the double-gyroid phase over the double-diamond or double-primitive phase is due to the packing frustration associated with the nonuniformities of interfacial curvature and domain size. Based on self-consistent field theory (SCFT), we demonstrate that a delicately designed miktoarm star A'(A"B)<sub>5</sub> copolymer can stabilize double-diamond and double-primitive network phases besides double-gyroid[1-2]. A number of sophisticated mechanisms for stabilizing the networks are revealed, including amplified effect of spontaneous curvature originating from the cone shape of A-blocks, effect of combinatorial entropy associated with the multiple A"B-arms and the effect of local segregation between the long A' and short A"-blocks. Under the synergistic effect of these three sophisticated mechanisms, the concentrations of the A' and A"-blocks in the nodes and struts are regulated by tuning the architectural parameters, thus controlling the sizes of the node and strut to match the geometry of various network structures. In brief, the A'(A"B)<sub>5</sub> copolymer with ingeniously tailored architectures can adopt two largely different forms of conformations to adapt to the local geometries of the node and strut of these three bicontinuous network phases, thus stabilizing them.

For the continuous network phase, another mysteriousness lies in why the double-gyroid phase but not the single-gyroid phase is often formed. Our SCFT calculations predict that the single-gyroid phase can be stabilized in a linear BABAB pentablock copolymer melt with proper block ratios and composition [3]. In this talk, we are also going to discuss about the stabilization mechanism of singlegyroid over double-gyroid [4].

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# Novel Tricontinuous Microphase-Separated Structures formed from ABC Triblock Terpolymer Blends

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It is well-known that non-gyroid cocontinuous structures is hardly constructed in block copolymer system, and a lot of investigation were carried out experimentally and theoretically so far.[1, 2] In this study, a double-primitive (DP) tricontinuous structure has been observed in a quaternary blend system consisting of two kinds



**Figure 1.** Schematic illustrations of the two ISP triblock terpolymers, I- and P-homopolymer investigated. Black, dashed and gray chains represent I, S, and P, respectively.

of ABC triblock terpolymers and A and C homopolymers (ABC'/A'BC/A/C) as illustrated in Figure 1. The two ABC triblock terpolymers have a chain length difference in the end block components, and the A/C homopolymers have comparable chain lengths with the longer A/C blocks of ABC triblock terpolymers.

Polyisoprene-b-polystyrene-b-poly(2-vinyl pyridine) (ISP) triblock terpolymers and I, P homopolymers were synthesized by a living anionic polymerization. The two ISP triblock terpolymers are approximately equal in total molecular weight ( $M_w = 120k$ ) and volume fraction of the middle block component ( $\phi_S = 0.6$ ). The two end block components I and P have a chain length difference of 5.8 and 6.8 folds, respectively.

Sample	$10^{-4} M_{n}^{a}$	$M_{\rm w}/M_{\rm n}^{\rm a}$	$\varphi_{I}:\varphi_{S}:\varphi_{P}^{b}$
ISP-α	10.9	1.02	0.35:0.60:0.05
ISP-β	12.2	1.02	0.06:0.62:0.32
1	4.9	1.05	-
Р	4.1	1.05	-
ISP-α/β/I/P	-	-	0.31:0.42:0.26

<sup>a</sup>Determined by GPC and GPC-MALS, <sup>b</sup>by <sup>1</sup>H NMR.

Figure 2(a) shows the transmission electron microscopy (TEM) image of the blend sample, ISP- $\alpha/\beta/I/P_{(0.31/0.42/0.26)}$ . This observed image was in good agreement with the simulated image for DP structure as shown in Figure 2(b). Furthermore, three-dimensional reconstructed image from TEM tomography (TEMT) showed a clear network structure of 6-fold branching as shown in Figure 3.



**Figure 2.** (a)TEM image of ISP'/I'SP/I/P, and (b)simulated image of DP(011).



**Figure 3.** (a)3D reconstructed image of ISP'/I'SP/I/P, and (b)6-fold branching point.

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# How Do You Make a Gyroid Chiral?

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Among the intriguing bicontinuous self-assembled structures, the gyroid cubic is the most ubiquitous. It contains two interpenetrating networks of opposite chirality and is thus achiral if, as usual, the content of the two nets is the same (Figure 1a) [1]. However we now find that strongly chiral compounds can also form the gyroid cubic structure, but a chiral one instead. While achiral molecules follow the opposite twists of nets 1 and 2 in the gyroid structure, molecules with a chiral center in their rod-like core do not follow the 70° twist between junctions in net 2 and instead wind against it by -110° to still match the junction orientation [2]. The metastable chiral gyroid is a high-entropy high-heat-capacity mesophase. The homochirality of its nets makes its CD signal close to that of the stable chiral bicontinuous cubic (space group I23) phase with 3 isochiral nets [3]. The relationship of this supertwisted chiral gyroid mesophase to other bicontinuous mesophases, as well as other ways of forming and modifying the gyroid phase in both chiral and achiral compounds, will be discussed too.



Figure 1: Models of a gyroid unit cell using spine-and-ribs ribbons, each rib representing a raft with molecules parallel to rib. (a) Achiral and (b) chiral gyroid. The "supertwisted" net in (b) is shown in purple.

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## **Gyroid Minimal Surface as Proton Conduction Pathway**

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Bicontinuous cubic (Cub<sub>bi</sub>) phase is a kind of nano-segregated liquid-crystalline (LC) phases in which both of two incompatible molecular parts form 3D continuous domains.<sup>[1]</sup> It has been found that Cub<sub>bi</sub> phases appear between lamellar and columnar phases both in the case of lyotropic liquid crystals and thermotropic ones. The volume balance between the two incompatible parts is one of the critical parameters for designing liquid crystals forming Cub<sub>bi</sub> LC assemblies. To date, we have focused on ionic liquid crystals having zwitterionic headgroups.<sup>[2,3]</sup> For example, we designed and synthesized pyridinium-based amphiphiles having zwitterionic headgroups. Although it forms only layered smectic phases in the pristine states, it co-organized into Cub<sub>bi</sub> LC phases in the presence of bis(trifluoromethane)sulfonimide (HTf<sub>2</sub>N).<sup>[3]</sup> It can be explained by the formation of ion pairs between the pyridinium zwitterion part and HTf<sub>2</sub>N through an ion exchange and the increase of the volume of the ionic parts. The Cub<sub>bi</sub> LC assemblies have a hydrophilic gyroid minimal surface where sulfonate group sit on densely and periodically. When a suitable amount of water is added to the Cub<sub>bi</sub> LC assemblies, a 3D continuous water nanosheet is created, which function as proton conduction pathway.



Figure 1. Induction of bicontinuous cubic phases for amphiphilic zwitterions.

Based on the molecular design of the amphiphilic zwitterions, we have recently succeeded in the development of a gemini-type amphiphilic zwitterion monomer forming  $\text{Cub}_{bi}$  phases.<sup>[4]</sup> UV irradiation for the monomer in  $\text{Cub}_{bi}$  phases leads to the formation of self-standing and insoluble polymer films with preserving the gyroid nanostructures. The polymer film shows quite high proton conductivity in the order of  $10^{-2}$  S cm<sup>-1</sup> in the H<sub>2</sub>O-absorbed condition.



Figure 2. Design of gyroid nanostructured polymer films using a polymerizable amphiphilic zwitterion.

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## Control of $Ia\overline{3}d$ Gyroid phase formation in aryloyl-hydrazine-based molecules by using two chemical modifications, introducing the side group and slight non-symmetry into the core moiety

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Control of the formation of  $Ia\overline{3}d$  Gyroid phases and their nano-structures is critical to advance Gyroid materials chemistry. In the thermotropic liquid crystalline (LC) systems, antispindle shape favors the  $Ia\overline{3}d$  LC phases, where both ends of the molecules, which are slightly expanded as compared to the central portion, causes the packing frustration on the side-by-side arrangement, resulting in the formation of two helical networks of opposite chiralities (ref. 1,2) (Figure 1). We have been investigating how various chemical modifications in the core portion of networks by side-by-side arrangethe aryloyl-hydrazine-based molecules change the thermotropic phase behavior (ref. 3).



Figure 1 Schematic illustration for the formation of two helical ment of antispindle-shaped molecules (ref. 1,2).

In this presentation, we two reveal chemical modifications in the core portion, introducing slight non-symmetry into the core portion (in 2-5) and attaching the methyl side-group (in 3-5), effectively lower and extend the  $Ia \ \overline{3} \ d$  phase regions, and change the core aggregation mode from the double-layered core (in 1 and 2) to the single-layered core modes (in 3-5), as revealed by the X-ray diffraction



Figure 2 Structures and phase transitions of four aryloyl-hydrazine-based molecules 1-5 (R = C<sub>22</sub>H<sub>45</sub>) on heating;  $I2_13$ , the so-called  $Im\overline{3}m$ -type chiral phase (ref. 4); Sm, smectic; Colh, hexagonal columnar phase. The electron density maps [green (medium) to red (high)] for the  $Ia\bar{3}d$  phases indicate two core aggregation modes.

intensity analyses (Figure 2). We discuss that the methyl group can control and tune the intermolecular cohesive interaction governing the formation of the  $Ia\overline{3}d$  LC phases.

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# Fitting into and shifting symmetries of block copolymer cubic networks

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Triply-periodic network morphologies constitute "natural forms" of self-assembled soft matter, forming in nearly every class of amphiphilic molecular building blocks, from surfactants and lyotropic liquid crystals to complex shape amphiphiles [1]. By far the most commonly observed network structures are the cubic domain networks: the double-gyroid (DG), double-diamond (DD) and double-primitive (DP). Their global structure reflects a "hybridization" between cylinders and layers, with one domain forming a double network of interconnected tubes (e.g. meeting at 3-, 4-, and 6-valent connections for DG, DD, and DP respectively), interspersed with a slab-like matrix layer, whose undulating shape approximates a triply-periodic minimal surface.

In this talk, I describe recent advances in the ability to connect the thermodynamic principles of self-assembly of block copolymer melts to geometric features of triplyperiodic double network morphologies. First, I describe a direct link between the medial geometry of double-[2], molecular networks configurations and the selection of the equilibrium DG phase in block copolymer melts, resolving a longstanding puzzle about the



**Figure 1** (A) "Slice & view" SEM tomography of continuous inter-phase transformation between DD and DG phase in polydimethylsiloxane-b-polystyrene block copolymers [7]. (B) Free energy landscape of tetragonal transformation pathway between DD and DG in strongly segregated diblocks.

strong-segregation phase behavior of networks [3]. This theory shows that among cubic double networks DG is unique in terms of the terminal packing geometry of chains, which is characterized twisted and "corner-free" weblike surfaces threading within tubular domains, accounting for a particularly large chain entropy and a window of thermodynamic stability [4]. Next, I describe efforts to understand the multi-scale morphology of block copolymer double networks distorted from cubic symmetry, motivated by recent in 3D tomographic studies or block copolymer double-networks that show prominent, yet coherent, symmetry-breaking distortions are the rule, rather than the exception [5]. These studies reveal a novel mechanism for non-affine collective rearrangements nodes and struts in acubic networks, which can be largely captured by a geometric principle of length-minimizing "liquid networks" [6]. Last, I describe recent studies of direct and continuous transformations between cubic DD and DG phases (Fig. 1) [7]. While it has long been known that DD phase is not equilibrium in a the phase diagram of linear diblock copolymer melts, we show the surprising result that DD is *not even metastable* and is generically unstable to DG via an non-affine tetragonal distortion pathway.

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# "Challenging" Steiner's formula: Pathways to stabilize the gyroid in colloidal self-assembly

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Mimicking assembly processes of highly complex and functional bicontinuous cubic phases (BPC) found in living organisms still marks a challenge in bio- and soft matter physics. Despite the first synthetically created BPCs being reported in the 1960s their scalability and orientability still fall short of nature's efficiency. In pursuit of novel methods for producing BCPs, I present a stabilization



**Figure 1** Particle arrangements within the gyroid phase (a) of pearshaped colloids (b), lipids in water (c), and di-block copolymers (d). At the bottom are the effective shapes of the pears (e), lipids (f), and di-block copolymers (g) within the curved bilayers [1].

mechanism for gyroid structures in colloidal self-assembly, that features collective packing rules to obey Steiner's formula. Using computational simulations of purely repulsive, nonadditive pear-shaped particles, Ι demonstrate that the colloids organize into interdigitated sheets with negative curvature, leading to the Gauss formation of gyroids [1]. Furthermore, the shape sensitivity of the stability of the gyroid phase reveals an underlying two-step assembly mechanism. fundamentally distinct from those observed in both lipid-water and diblock copolymer systems [2].

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## Magnetism and topology in self-assembled 3D gyroid nanostructures

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Gyroids are renowned in the fields of metamaterials and photonics for their connectivity and chirality, and are now beginning to draw their due attention in the field of magnetism. I will describe our work on the fabrication of magnetic gyroids with node-node distances close to the magnetostatic exchange length, and our work on imaging their magnetic states via electron holography [1]. Our attempt to provide a framework to understand the magnetization dynamics of a small number of gyroid unit cells [2], and how their interactions may generate and influence spin waves [3] is described. Finally, I will touch upon the long-range ordering of gyroids over tens to hundreds of unit cells, including ways to control the morphology by directed self-assembly [4]. I will explain how ptychographic X-ray computed tomography (PXCT) was employed for large-scale observations of gyroids and the related single-diamond network at sub-unit-cell



Figure 1 Representation of the intricate configuration of the magnetization in nanoscale magnetic gyroids

resolution, and how this technique enabled us to reveal the existence of topological defects which arise during self-assembly [5].

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## Structural transformation of cholesteric blue phases revealed by continuum simulation and machine-learning-aided structural analysis

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Cholesteric blue phases of a chiral liquid crystal [1] have been known as intriguing examples of exotic three-dimensional ordered structures exhibited by soft materials. They comprise a regular array of disclination lines (line defects of orientational order) and double-twist cylinders in which the orientational order is twisted along all the directions perpendicular to the cylinder axis. Two blue phases, BP I and BP II, show cubic order, and BP I has the space group  $I4_132$ , the same as that of a single gyroid (The space group of BPII is  $P4_232$ ). The transition between BP I and BP II is an interesting example of transformation between ordered structures.

When a perfect lattice of BP II is cooled, it exhibits first-order phase transition to BP I. Recent experiments [2] revealed the formation of twinned structures that resembles those observed in martensitic transformation. However, the real-space dynamics of the transformation is still unclear. Here we carry out a simulation based on a Langevin-type equation for the dynamics of orientational order parameter, a second-rank tensor. The complex ordering of BP I and BP II makes the identification of local structures a non-trivial task. We overcome this difficulty by supervised machine learning that successfully distinguishes BP I and BP II.

Figure 1 shows a snapshot of simulation with a BP I nucleus. We emphasize the difficulty of identifying the BP I region by the structure of the disclination network alone. Further growth of the



**Figure 1** A snapshot of simulation exhibiting the formation of a BP I nucleus (magenta) Gray lines are disclinations forming BP II.

nucleus is shown to lead to the formation of well-defined twin boundaries between BP I regions with different lattice orientation. We also find that by raising the temperature the twinned BP I structure almost reversibly recovers the perfect BP II ordering. Our simulation study with machine-learning-aided structure analysis successfully clarifies the transformation dynamics of blue phases involving twin boundaries, and will be applicable to other problems on complex structural transformation between ordered phases exhibited by a wide variety of soft materials.

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## Topological electronic states in microscopic gyroids

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The gyroid is a three-dimensional periodic structure that has been realized in various systems and scales [1]. It has been demonstrated that the photonic gyroid crystal exhibits topologically nontrivial band structures, including Weyl points and line nodes, which reflect the high symmetry of the structure [2]. In this study, we focus on the electronic properties of the microscopic gyroid structure to explore the unique topological features arising from the symmetry of the crystal structure.

The chiral crystal structure known as the "single gyroid" has a configuration where each lattice point is connected by three bonds [Fig. 1(a)]. This single gyroid structure is one of the structures with the highest symmetry, referred to as "strong isotropy," along with honeycomb and diamond structures [3]. Due to its high symmetry, the higher-spin Dirac points can appear at the  $\Gamma$  point in the electronic band structure of the single gyroid [4]. Although the synthesis of a single gyroid with carbon atoms has not been successful to date, the synthesis of a single gyroid structure using organic molecules has been achieved, and the realization of a spin liquid has been confirmed [5].

In the present study, we focus on the nested crystal structure consisting of two single gyroids, known as the "double gyroid" [Fig. 1(a)]. Figure 1(b) shows the electronic band structure based on the tightbinding approximation considering only a single orbital at each site. Unlike the single gyroid, the double gyroid exhibits accidental degeneracy between the conduction band and the valence band. A detailed analysis of this degeneracy revealed that the bands degenerate continuously within the threedimensional momentum space, forming what is known as a "Dirac line node" [Fig. 1(c)]. The Dirac line nodes in the double gyroid, unlike the loop-like line nodes previously discovered, are open across the Brillouin zone and form a total of 12 line nodes within the Brillouin zone [Fig. 1(d)]. In the presentation, we will further discuss the topological properties associated with these unique band structures.



**Figure 1** (a) Double gyroid structure. The space group is Ia $\overline{3}$ d (No. 230). The brown and purple structures represent single gyroid structures. (b) Band structure of the double gyroid structure. The nearest-neighbor hopping is set to  $t_0=0.5$  and the next-nearest-neighbor hopping is set to  $t_1=1$ . (c) Dispersion relation of the Dirac line nodes. (d) Dirac line nodes in the Brillouin zone.

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## **Coexistence of Collinear and Non-collinear Spin Texture in Antiferromagnetic Gyroidal MOFs**

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The gyroid structure is a three-dimensional periodic structure with high symmetry and chirality discovered by A. H. Shoen [1] and has attracted much attention in a wide range of fields including chemistry, physics, mathematics, and architecture. We have also provided a rational explanation using line graphs in graph theory for "hidden geometrical frustration" in the gyroidal molecular assembly: when antiferromagnetic spins are present at the midpoints of the vertices of a single gyroid lattice, the resulting spin configuration forms a hyper-kagome lattice known as a spin frustration lattice to have the quantum spin liquid state. [2].

Metal-organic frameworks (MOFs), in which organic ligands interconnect metal centers, are excellently designed systems to show the attractive properties of a gyroid lattice (Fig. 1). The chemical diversity of ligands and the unique topologies of lattices make MOFs highly attractive for research. For instance, our recent findings highlight that the chirality of the single gyroid lattice in the  $[Ru(bpy)_3][M_2(ox)_3] (M = Zn, Mn,$ bpy = 2.2'-bipyridyl, ox = oxalate) significantly enhances the solid-state circularly polarized luminescence of Ru(bpy)<sub>3</sub><sup>2+</sup> luminophores due to the host-guest interactions [1]. Furthermore, we unveiled that the gyroidal MOF with local magnetic anisotropy  $[Ru(bpy)_3][Co_2(ox)_3]$  causes exchange frustration resulting in the emergence of various quantum magnetic states [4].

What spin configuration would result if the antiferromagnetic spins were placed at the vertices of a gyroid lattice? This question motivated us to carry out the magnetic structure analysis of the single gyroidal MOF  $[Ru(bpy)_3][M_2(ox)_3]$  (M = Mn, Co) using the single-crystal neutron diffraction (Fig. 2). Forbidden reflections derived from magnetic scattering were observed in the antiferromagnetic phase at low temperatures. Detailed analysis of these peaks revealed that the Mn sites split into two sites in the low-temperature phase, forming the coexistence of collinear and non-collinear spin textures.



Figure 1 The possible spin texture in antiferromagnetic gyroidal MOFs.



Figure 2 Neutron diffraction images.

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## **Gyroid Photonics – From Chiral Beamsplitters and Active Materials to Topological Physics and Bound States in the Continuum**

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In this lecture, I will explore the breadth of photonic effects associated with nano-structured gyroid materials. I will focus on optical composites, where one (chiral single gyroid) or two (achiral double gyroid) of the gyroid's network channels are filled with constituent optical materials [1]. As a common theme, we will find that the network topology and material fill fraction govern the light-matter interaction. On the other hand, the specific geometrical realisation – for example, constant mean

curvature domains or rod-connected networks – only weakly affects the photonic response.

Most photonic nano-composites are classified as *photonic crystals* (PhCs) or *metamaterials* (MMs). PhCs are dielectric structures whose optical properties are primarily obtained from an interference effect caused by a refractive index variation on the order of the wavelength of the light. PhCs started to attract attention after two seminal papers appeared in the same issue of Physical Review Letters in 1987, describing strong Anderson localisation of light (S. John) and completely suppressed spontaneous emission (E. Yablanovitch). Both effects have



**Figure 1** Towards active gyroid media. A biotemplate (A) is infiltrated with a barium-titanate sol-gel (B) to obtain a nonlinear PhC, or cast into an active metamaterial through (C) atomic layer deposition, (D) electrodeposition, (E) etching of the biotemplate, and (F) infiltrating with a dye or quantum dot solution. Reproduced from [2].

not been experimentally demonstrated to date. I will explain why a gyroid PhC infiltrated with an active photonic component, illustrated in Figure 1, is an excellent candidate to test and exploit Yablanovitch's hypothesis. But even without an active component, gyroid PhCs offer many exciting phenomena. For example, the single gyroid's 3D chirality has been exploited to design a circular polarisation beamsplitter, as shown in Figure 2. On the other hand, a double gyroid PhC with broken parity symmetry was the first practical physical system in which the Weyl equation could be demonstrated 85 years after

its derivation by Ling Lu and coworkers at MIT.

Gyroid MMs are metallic composites typically structured on a sub-wavelength scale. They obtain their optical properties from how the 3D gyroid topology restricts the plasmonic excitations of the free electrons in the constituent metal. Gyroid MMs based on block-copolymer self-assembly have long been considered an ideal candidate to achieve 3D negative refraction and build Pendry's *perfect lens*, with a resolution not limited by diffraction. I will



of the fabricated device. Reproduced from [3].

explain the failure of attaining negative refraction in single gyroids and highlight the potential of double gyroids MMs as a 3D lasing cavity through a bound state in the continuum mechanism.

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### **Functional Morphology of Mesoscale Organismal Single Gyroids**

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A rich diversity of complex three-dimensional photonic nanostructures produce vivid interference colors in the integument of many animals that are used prominently in communication and camouflage. Such fade-proof, saturated structural colors that have evolved over millions of years of selective optimization are an ideal source to look for natural solutions to our current technological challenges in optics, and sensing. Using synchrotron Small Angle Xray Scattering (SAXS), we have unambiguously elucidated the 3D nanoscale organization of biophotonic nanostructures across hundreds of species and discovered the enigmatic single network gyroid photonic crystals within wing scales of butterflies (ref. 1) and beetles (ref. 2), and more recently in the feather barbs of certain leafbirds (ref. 3) (Figure 1). Insects appear to grow these nanostructures by the complex invagination of lipid bilayer membranes with associated cuticle in a templated fashion that is eerily reminiscent of current engineering approaches and rivals the phase behavior of amphiphilic or lyotropic macromolecules but at the hard to achieve visible optical length scales. Whereas leafbirds (Figure 1) appear to develop visible optical or meso-scale single



**Figure 1** Evolution of single gyroid photonic nanostructures in the feather barbs of Blue-winged Leafbird from ancestral quasi-ordered spinodal-like morphologies found in sister species (see ref. 3).

gyroids in a bottom-up fashion directly via phase separation of feather keratins - a process that has no parallel in either physics or biology. We will juxtapose the comparative development of keratinaceous vs. chitinaceous single gyroids and discuss how the self-assembly of biosimilar patchy particles with both short-range attraction and long-range repulsion (akin to the keratins in developing feather barbs) could be the answer to unlocking facile biomimetic routes to materials synthesis at the challenging optical length scales for advanced functional applications from sensors, photonics, energy harvesting to catalysis.

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## **Beyond the Ordinary: Diamond- and Gyroid-Shaped Membranes in Plant Plastids**

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<sup>1</sup>Department of Plant Anatomy and Cytology, Institute of Experimental Plant Biology and Biotechnology, Faculty of Biology, University of Warsaw, Miecznikowa 1, PL-02-096 Warsaw, Poland <sup>2</sup>Times New Roman Italic 10 pt

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Cellular membranes exhibit the remarkable ability to self-organize into diverse morphologies. Among these, bicontinuous membrane (so called cubic membranes) stand out as the most complex periodic arrangements, characterized by a fascinating interplay of biological form and geometry. These cubic membranes share structural similarities with triply-periodic minimal surfaces, especially those of primitive, diamond and gyroid-type. While such intricate membrane structures have been observed in various organisms, from protozoa to mammals, our understanding of the structural and molecular mechanisms governing their formation and subsequent transformation into other membrane shapes remains limited. Due to the lengthscale of cubic membranes (around 50-500 nm) and their fluid nature, 2D and 3D transmission electron microscopy (TEM) is the analysis method of choice to decipher their nanostructural features.

In our research, we employ plant plastids' internal membranes as a model system to explore cubic morphologies. Plastids, a diverse group of organelles found in different plant organs, serve various functions closely tied to their inner membrane networks, with photosynthesis being a prominent role. By investigating the interplay between structure and composition in self-organizing cubic and lamellar arrangements during plastid ontogenesis, we aim to decipher how changes in membrane composition impact the formation and stability of these unique membrane assemblies.

During my presentation, I will delve into our approach for recognizing and annotating cubic assemblies using the SPIRE software tool [1]. SPIRE facilitates the identification of bicontinuous membrane structures from TEM sections by interactive matching against mathematical "nodal surface" models. I will also describe the specific features, assembly mechanisms, and biological function of two physiologically important examples of cubic membranes in plant plastids - the Diamond-shaped prolamellar body of the etioplast occurring naturally during plant development and Gyroid thylakoid assembly transiently present in fully developed and photosynthetically active chloroplast (Figure 1).



Figure 1 Figure legend. (Times New Roman, 9 pt)

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# Reflections from a developing butterfly Gyroid

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The occurrence of single Gyroid nanostructures in butterflies is remarkable; not least because of the large unit cell sizes (~300 nm) that allow the structures to behave as three-dimensional biophotonic crystals. The single Gyroid structure has been found in several species of butterflies, generating a striking green coloration. While Gyroid structures have been well documented in other naturally occurring systems, the sizes of the structures found in butterflies are much larger, leading to the question of their formation. In butterflies, single Gyroid nanostructures are found within the lumen of their wing scales. Each scale develops from a single cell whose plasma membrane acts as a template to the nascent chitin, forming elaborate nanostructures. Upon maturation, the scale cell dies and recedes leaving only the chitinous nanostructures. In the butterfly Callophrys gryenus, the complex Gyroid network is thought to be templated by an additional intracellular membrane, namely the smooth endoplasmic reticulum (SER). This membrane, along with the plasma membrane are thought to fold into a double Gyroid geometry comprising three distinct channels: the extracellular space, the intracellular space, and the intra-SER space. The prevailing hypothesis is that chitin is deposited into this extracellular space, thereby generating a chitinous single Gyroid structure, and that the remaining channels are filled with cytoplasm and extracellular fluid that are gradually replaced by air as the scale cell recedes [1,2]. Currently, the only evidence to support this hypothesis comes from Ghiradella's seminal TEM study of fixed pupal wing tissue from different developmental stages [3]. The lack of evidence is largely due to the difficulties associated with imaging structures of this size. Their nanometer scale limits imaging techniques to electron microscopy which restricts the sample to one that can be imaged under vacuum (i.e. not a living organism). What is needed to understand the details of the formation mechanism is a technique that allows in vivo imaging of a developing butterfly pupa.

Here, we take advantage of the fact that these structures are photonic and measure the reflections that are generated by developing biophotonic Gyroid nanostructures in *Parides sesostris* to infer specific details about their development. We developed and used a hyperspectral microscopy method [4] and electron microscopy to show that the Gyroid nanostructure begins to generate red-shifted reflections peaking ~610 nm at ~75% development. Over the course of ~48 hours these reflections grow and almost triple in amplitude. These red-shifted reflections are commensurate with optical models of a chitinous single Gyroid nanostructure that is embedded within a cytosolic medium and provide further support for the double Gyroid templating hypothesis.

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# A Single Grain of OBDG in a Semi-dilute Solution - Photonic Crystal

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Many researches and inventions of non-linear optical material have been stimulated for these decades by the publications on the optical properties of three-dimensionally arrayed dielectric materials by Yablonovitch and John in 1987. The optical materials allow us to control the flow of light, providing a new technology for optical devices, such as low-energy consumption laser resonators, high-speed computers, light storage, and so on.

We have succeeded in the fabrication of a photonic crystal (PhC) by self-assembly of block copolymers (BCP) that generally form one-, two-, and three-dimensional periodic nanostructures, i.e., lamellar, cylindrical, spherical, gyroids microdomains, etc. Lattice spacings of the microdomain structures depend on the molecular sizes of BCPs. To obtain a large spacing on the order of the wavelength of visible light, we should utilize BCPs with ultra-high-molecular weight (UHMW), such as 10<sup>6</sup> g/mol. They, however, are highly entangled and, hence, too viscous in bulk to attain structural equilibrium. Even in a semi-dilute solution at several percent, we have found that solvent selectivity strongly induces microphase separation (Fig. 1) [1,2]. BCPs can easily form equilibrated structures with high order at such low concentrations because of their high mobility. Large grains on the order of centimeters (Fig. 2) were obtained in the vicinity of the boundary of the lyotropic order-disorder transition. These phenomena were well analyzed by computer simulation using "SUSHI" [3,4].

We have successfully applied these structures in a THF/water mixture to a laser resonator. The specimen utilized here was a ultra-high-molecular-weight polystyrene-*b*-polymethylmethacrylate diblock copolymer, forming ordered-bicontinuous double gyroid with a tris octahedron structure. They successfully inhibit the spontaneous emission of dyes, and laser emission was generated in twenty four directions as seen in Fig. 3. The laser threshold was  $0.1 \mu$ J/pulse and is dependent on the refractive index difference between the phases, i.e., the reflectivity, and the number of the stacked lattice planes. In this paper, we will discuss the resonator efficiency as a function of reflectivity and grain size, and also a new possible pathway to realize metamaterials.



Figure 1 Microphase separation induced by selective solvent

**Figure 2** a giant grain in a BCP solution.

**Figure 2** Laser emission from microdomain sturctures

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# **Rational Synthesis of Molecular Gyroids and their Structure-Derived Solid-State Properties**

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A.H. Shoen discovered the gyroid, an infinitely-connected triply-periodic minimal surface that separates 3D space into a pair of enantiomorphic channels called single gyroids [1]. These gyroidal structures are ubiquitous in nature, appearing in various materials of different sizes. In fact, the gyroidal structure can be formed by atoms and bonds, corresponding to space discretization in geometry, as well as molecules and intermolecular interactions, and metal ions and ligands.

We have been working on the rational construction of gyroidal structures using polyhedral  $\pi$ -conjugated

molecules that consist of three  $\pi$  planes with normal vectors forming  $C_3$  symmetry. It was found that the electrochemical crystallization of NDI (naphthalene diimide)- $\Delta$  resulted in single crystals of (TBA)<sub>1.5</sub>[(-)-NDI- $\Delta$ ] (TBA = tetrabutylammonium), where (-)-NDI- $\Delta$  forms a chiral single gyroid lattice due to its triangular molecular structure and intermolecular  $\pi$ - $\pi$  overlap between the NDI moieties [3] (Fig. 1). The line graph consideration revealed that this lattice is identical to the hyper-kagome lattice of *S*=1/2 Mott dimers, exhibiting 3D spin frustration. Indeed, low-temperature magnetic and heat capacity measurements indicated the presence of a spin-liquid ground state [4,5].



Fig. 1. Molecular gyroid, formed by (-)-NDI- $\Delta$ .

Among microscopic gyroidal materials, the coordination gyroids, which consist of magnetic metal centers and ligands, have been explored for more than 20 years [2]. The gyroidal oxalate complexes are

the most investigated family due to their extensive magnetic properties. Recently, we examined the circularly polarized luminescence (CPL) for  $[Ru(bpy)_3]I_2$  (1) and  $[Ru(bpy)_3][M_2(ox)_3]$  (M=Zn (2) and Mn (3)). Whereas Compound 1 is a simple salt of  $[Ru(bpy)_3]^{2+}$ , 2 and 3 are the MOFs in which the chiral  $[Ru(bpy)_3]^{2+}$  ions are encapsulated in a homochiral gyroidal skeleton of  $[M_2(ox)_3]^{2-}$ . Whereas the solution of 1 exhibited a weak CPL with a luminescence dissymmetry factor of  $|g_{lum}|\sim 10^{-4}$ , the CPL was significantly enhanced in the solid-state  $1\sim 3$  with  $|g_{lum}|=2x10^{-2}$  for 1,  $4x10^{-2}$  for 2, and  $1x10^{-1}$  for 3. The enhanced CPL in 3 was attributable to an energy transfer between the homochiral guest and host in 3 [6] (Fig. 2).



Fig. 2. Enhanced CPL in gyroidal oxalate complexes.

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Poster P1-1 15:20-17:20, November 20 (Wed)

### Unknotting 3-periodic entanglements of filaments and nets

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Entanglements of curves and nets can be found in various biological and chemical structures, such as in coordination polymers, in liquid crystals, or in DNA origami crystals. One example is the crystal structure of cyanamide NH<sub>2</sub>CN, that can be regarded as the interpenetration of two enantiomorphic srs nets [1].

New diagrammatic descriptions of 3-periodic entanglements have been recently defined in [2]. These new diagrams are drawn out of a projection along one axis of a unit cell of a 3-periodic structure. Three projections along three non-coplanar axes constitute a *tridiagram*. It has been proven in [2] that tridiagrams fully encode ambient isotopies of 3-periodic structures, as long as the isotopies preserve the periodicity. The notion of tridiagram allowed the definition of the crossing number for 3-periodic entanglements.



Figure 1 A unit cell of two enantiomorphic srs nets as they sit in the channels of the gyroid



Figure 2 One diagram drawn from a projection of the unit cell of Figure 1

By using tridiagrams, we wish to extend the notion of *unknotting number* to the 3-periodic setting. We do so by listing some conditions required to transform a structure to another, whose crossings cannot be eliminated by an unknotting operation. We illustrate the practicality of this extended unknotting number on various examples of 3-periodic entanglements of curves and nets. The extended unknotting number exhibits the difference between a given embedding and the "least knotted" embedding, and the relation between them.

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Poster P1-2 15:20-17:20, November 20 (Wed)

## Macro scale gyroid applications

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The gyroid TPMS discovered by Schoen in 1970 (ref. 1) is a fundamental building block which self-assembles at nano scale (ref. 2). It is found at nano scale in plant and animal kingdoms, as well as at micro scale in sea urchins (ref. 3). The gyroid surface divides 3D space into two interlocking spaces and exhibits high surface to volume ratio. Flow through each of the two spaces branches repeatedly, with a left-hand spiral branch and a right-hand spiral branch at each intersection.

The elegant complexity of the gyroid structure has made it difficult to reproduce at macro scale. As 3D printing processes have improved, the gyroid has become a popular infill, reducing weight while maintaining structural stability, and self-supporting during the printing.

Using numerical analyses and 3D printing, gyroid structure has been proved useful at millimeter scale for processes requiring countercurrent flow (e.g.: active heat exchange (ref. 4), mass transfer), and for mechanical properties of objects that require both strength and reduced weight (e.g.: passive heat exchange, packaging, bone replacement). At larger scale, architectural uses have been suggested (e.g.: wall, bridge). A relatively straightforward method of assembly is described for creating gyroid structure using traditionally manufactured parts (cast, milled, injection molded, etc.).



Figure 1 Gyroid pipe assembled from 10 skew hexagons.

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Poster P1-3 15:20-17:20, November 20 (Wed)

# **Discrete Gyroid Structures: Defect-Driven Tiling and Analogies with Zeolite Frameworks**

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This presentation explores the connection between discrete gyroid structures with defects and the framework of zeolite structures. Both structures exhibit complex topologies and periodic characteristics that are of interest in materials science.

Gyroidal structures, discovered by Alan Schoen in 1970, are known for their continuous, non-selfintersecting surfaces that divide space into two interpenetrating labyrinths. These structures are notable for their minimal surface properties, making them an intriguing subject of study in both theoretical and applied sciences. Beyond their continuous form, gyroidal structures can also be discretized. This process involves transforming the smooth surface into a network of discrete points or tiles, which allows for easier computational modeling and practical application.

Our approach to discretizing gyroidal structures starts from regular tiling (planar tiling). By introducing defects into these regular tilings, we can describe the gyroidal surface in a more controlled manner. This method allows us to connect the polygons used in tiling with the Euler-Poincaré formula, providing a quantitative relationship between the number of polygons and the genus of the surface. Regular tiling typically involves three types of polygons: triangles, squares, and hexagons. Among these, triangles and hexagons are dual to each other, and the use of hexagons has been previously discussed in the context of Chern-Chuang's work [1]. Therefore, our focus in this study is on square tiling.

To ensure that the tiling can adhere to a curved surface, it is necessary to use squares along with defect hexagons. This combination ensures that each vertex in the tiling is tetravalent (4-degree). Moreover, zeolites have a silicon atom framework where each silicon atom is connected to four oxygen atoms, forming a tetrahedral network. This tetravalent connectivity leads to a wide variety of zeolite structures, many of which share similarities with gyroidal structures such as BSV and ANA, demonstrating their relevance and applicability.



Figure 1 Structure diagram of zeolite BSV. (a) highlighting hexagonal defects. (b) highlighting ribbons formed by squares, colored to distinguish left- and right-handed helices. (c) Top view of (b) showing the hollow space formed by helices.

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### **Construction and Classification of Hyperbolic Diagrams and their Triply Periodic Weavings & Polycatenanes via Mapping to the Gyroid** Sonia Mahmoudi<sup>1,2</sup>

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This poster presents a framework for studying the topology of triply periodic tangles embedded in the thickened gyroid, referred to as *G-TP tangles*, which play a key role in materials science and chemistry. G-TP tangles arise, for example, in self-assembled materials, where the relationship between structure and functions is influenced by the underlying topology. The thickened gyroid serves as a periodic scaffold, making it ideal for modeling molecular structures and polymeric systems.

Some G-TP tangles can be related to graphs on the hyperbolic plane, where hyperbolic tilings are mapped onto triply periodic minimal surfaces (TPMS) using the symmetries and periodicities inherent in hyperbolic space to embed entangled structures into the gyroid scaffold [1], as illustrated in Figure 1.



Figure 1. A tiling of the hyperbolic plane, its mapping a fundamental domain of the gyroid and its G-TP tangle (from [1]).

In this poster, we extend this work by presenting a method for constructing and classifying G-TP tangles. We begin by considering a graph on a genus 2 surface  $\Sigma$ . Using the *polygonal link method*, we transform this graph into a link diagram on  $\Sigma$  [2]. By selecting appropriate characteristic curves, the link diagram is unfolded into a tangle diagram in a hyperbolic octagon, which is then lifted into a periodic tangle diagram on the hyperbolic plane, as illustrated in Figure 2. The above method of [1] is then used to map this periodic diagram onto the gyroid. Finally, this diagram can be lifted to the thickened gyroid, resulting in a G-TP tangle embedded in Euclidean 3-space. This study can be generalized to other TPMS.



Figure 2. A periodic tiling of the hyperbolic plane to which two different polygonal link methods are applied [2].

To classify these G-TP tangles, we use the *extended Jones polynomial* for link diagrams on  $\Sigma$  representing unit cells of periodic hyperbolic diagrams, as defined in [3]. To account for global isotopies of the G-TP tangles, invariance under Dehn twists on  $\Sigma$  is considered, which correspond to volume-preserving shearing of the G-TP tangles, as well as the choice of unit cells of different volumes.

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### **Curvature Estimation based on Distance Conversion of a 3D image**

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Surface curvatures has been of importance in understanding the complicated network structures. Nevertheless, it is not simple to measure the curvatures in the experimental systems. We has proposed two methods to measure the curvatures from the 3d images [1,2], and one more is also proposed by Lopez-Barron et al.[3]. All methods concerns the surface rendering process, and hence the "hard" binarization is necessary in advance to the surface rendering. Binarization usually accompanies *delicate* noise reduction. Therefore the less-noise 3d image is necessary for measuring accurate curvatures. Instead of that, we propose a new method based on distance conversion, which also needs the binarization but is rather insensitive to the noises. Furthermore, the method is theoretically applicable to other physical measurements, such as BET.

In the Parallel Surface Method (PSM)[1], the area of the parallelly-constructed surface (say, parallel surface) at distance t, S(t), is related to the mean (H) and Gaussian (K) curvatures as,

$$S(t) = S(0)(1 + 2Ht + Kt^{2}).$$
 (1)

Immediately, we can obtain the integration form of eq. (1) as,

$$V(t) = \int_0^t S(t)dt = S(0)\left(t + Ht + \frac{K}{3}t^3\right),$$
 (2)



Figure 1 Schematic illustration of V(t)

where V(t) is the volume between the original surface (t =

0) and the parallel surface at distance t. Figure 1 shows the schematic illustration of V(t). For simplicity fig. 1 shows the 2D case. In V(t), the distance to the original surface is less than t. In the digital images, the distance can be estimated via distance conversion [4]. Then now we obtain a new method to measure the surface curvatures for 3d images: (i) binarizing the image, (ii) applying the distance conversion, (iii) counting the voxels less than t and (iv) fitting thus obtained V(t) with eq. (2).

Since the distance conversion is slightly insensitive to the image noises, the new method is expected to be more robust than other methods. V(t) is essentially the volume of the layer of thickness t on the original surface, which can be obtained besides the 3d image processing. BET measurement is the one, in which an inert gas is condensed on the surface under high pressure. The thickness of the condensed gas layer is considered to be constant everywhere on the surface which is exactly same definition as V(t).

In the 3d image analysis version, we found that the method needs the stochastic correction. As seen fig. 1, some parts of the parallel surface often protrude the region of the image where are also necessary for V(t) but are not counted in the distance conversion. To correct this situation, we estimated the probability of V(t) outside the image are estimated and used in the fitting by eq. (2). The new method is critically examined by using model images including gyroid.

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# Design economy and assembly of size-programmable triply-periodic polyhedra from addressable nanotriangles

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As first suggested by Caspar and Klug [1], many viruses assemble icosahedral shells (capsids) because the high symmetry of the icosahedron enables economical assembly – enclosing a large volume with relatively few distinct protein subunit types. We propose and



Figure 1 Sequence of snapshots of simulated assemblies of T = 3 Gyroids from programmable triangular subunits, where colors indicate distinct subunit species.

investigate an extension of the Caspar-Klug symmetry principles for viral capsid assembly to the programmable assembly of size-controlled triply-periodic polyhedral [2], discrete variants of the Primitive, Diamond, and Gyroid cubic minimal surfaces [3]. Inspired by a recent class of programmable DNA origami triangular colloids [4-5], we demonstrate that the economy of design in these crystalline assemblies – in terms of the growth of the number of distinct particle species required with the increased size-scale (e.g. periodicity) – is comparable to viral shells. We further test the role of geometric specificity in these assemblies via dynamical assembly simulations, which show that conditions for simultaneously efficient and high-fidelity assembly require an intermediate degree of flexibility of local angles and lengths in programmed assembly. Off-target misassembly occurs via incorporation of a variant of disclination defects, generalized to the case of hyperbolic crystals. The possibility of these topological defects is a direct consequence of the very same symmetry principles that underlie the economical design, exposing a basic tradeoff between design economy and fidelity of programmable, size controlled assembly. We also present preliminary results of experimental efforts to realize Primitive assemblies from assembly of DNA origami colloids programmable edge binding and geometry.

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### **Exploring the Homogeneity of Disordered Minimal Surfaces**

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Bicontinuous geometries, both ordered and amorphous, are commonly found in many soft matter systems. For ordered phases with crystalline symmetry, periodic bicontinuous minimal surfaces provide established models, including Schoen's Gyroid and Schwarz's Diamond surfaces. Conversely, a minimal surface model for amorphous phases has been lacking. Here, we study models for amorphous bicontinuous phases, such as sponge phases. We use the Surface Evolver [1], with a novel topology-stabilizing minimization routine, to generate discretized minimal surfaces from initially coarse polyhedral meshes. We demonstrate that minimal companion surfaces to the amorphous Diamond network exist, providing a structural model for sponge mesophases.



As per Hilbert's Embedding Theorem, the Gauss curvature of any curved minimal surface cannot be constant. An

analysis of variances  $(\Delta K/\Gamma^2)^2$  of the Gaussian curvature [2] of both periodic and aperiodic surfaces reveals that the amorphous Diamond minimal surface has no substantial, interior long-wavelength curvature variations (see Fig. 2). However, the total variance of Gauss curvature for all considered amorphous minimal surface models is significantly larger than that of the cubic Diamond and Gyroid



**Figure 2** Curvature distributions of amorphous Diamond surface subsamples next to Gyroid deformation families.

Figure 1 Curvature variance and isotropy of several amorphous diamond surface subsamples, compared to known surface families.

r than that of the cubic Diamond and Gyroid surfaces (see Fig. 1). The functional form of the curvature distributions and the duality properties of the two labyrinthic components afford pertinent insight into the origin of curvature variations. We also consider these surfaces' isotropy indices  $\beta_1^{0,2}$  [3]. We find that the amorphous Diamond surfaces are highly isotropic (see Fig. 1), typically producing  $\beta_1^{0,2} > 0.95$  with  $\beta_1^{0,2} = 1$ corresponding to completely isotropic surfaces.

Our work demonstrates the degree to which the curvature homogeneity of the cubic Gyroid and Diamond surfaces is superior to

their entropy-favored amorphous counterparts. It thereby provides a general geometric result of relevance to bicontinuous structure formation in soft matter and biology across all length scales, relevant to both ordered and amorphous phases.

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## On characterizing the topology and geometry of imperfect gyroids.

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Triply periodic network morphologies are commonly found across various self-assembled soft matter systems, including diblock copolymers. Among these is the double gyroid phase, characterized by two distinct and interpenetrating tubular minority domains embedded within a majority domain whose shape approximates a finite-thickness gyroid minimal surface. In real systems, these crystalline double-networks often coexist with defective or disorder variants of the same networks. In this study, we exploit 3D tomographic restrictions of polystyrene–polydimethylsiloxane (PS–PDMS) diblock copolymer samples to examine boundaries between well-formed (that is, cubic) double gyroid networks and "aperiodic network" regions that tend to form in inter-grain regions. Despite the lack of long-range order in the aperiodic network, we find that it predominantly exhibits the same 3-valent tubular network connections as the ordered double-gyroid, but with a much more variable structure of looping. Using tools from network theory and geometry, we characterize the structure of the aperiodic regions. Through this analysis, we hope to uncover how aperiodic regions, consisting of a single network domain, transform into ordered double gyroids, comprising two separate network domains.

## **Cocoon Microstructures through the Lens of Topological Persistence**

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Biological materials display various functionality, often dictated by complicated microstructures. Studying the complex structure of silk-worm cocoons can give inspiration to new bio-mimetic engineering applications.

Developing of new geometric and topological strategies enables us to describe the microstructures precisely and systematically. The silkworm cocoon is an example of a complex microstructure, producing a complicated entangled material.

This poster on the microstructural analysis of *B. mori* silkworm cocoon using three-dimensional voxelised ( $\mu$ CT) scans. We approach this data through the lens of persistent homology to derive conclusions about pore size gradients and fibre thickness gradients. Analyzing the fiber alignments we demonstrate the uniform fiber orientations.

# **Programmable Self-Assembly of Nanoplates into Bicontinuous Nanostructures**

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Self-assembly is the process by which individual components arrange themselves into an ordered structure by changing shapes, components, and interactions. It has enabled us to construct a remarkable range of geometric forms at many length scales. Nevertheless, the potential of two-dimensional polygonal nanoplates to self-assemble into extended three-dimensional structures with compartments and corridors has remained unexplored. We show coarsegrained Monte Carlo simulations demonstrating selfassembly of hexagonal/triangular nanoplates via DNAmediated complimentary interactions into facetted, sponge-like "bicontinuous polyhedra" (or infinite polyhedra) whose flat walls partition space into a pair mutually interpenetrating labyrinths. of Two bicontinuous polyhedra can be self-assembled: the



**Figure 1** Infinite bicontinuous polyhedra. (a)  $\{6,4|4\}$  regular infinite polyhedron  $(Im\bar{3}m)$ . (b) Jungle-gym labyrinth. (c) The Primitive surface. (d, e) Two views of a "gyrangle", another regular infinite polyhedron  $(I4_132)$ . The gyrangle consists of four sets of parallel triangles. (f) The Gyroid surface  $(Ia\bar{3}d)$ .

regular (or Platonic) Petrie-Coxeter infinite polyhedron (denoted {6,4|4}) and the semi-regular Hart "gyrangle". The latter structure is chiral, with both left- and right-handed version. We show that the Petrie-Coxeter assembly is constructed from two complementary types of hexagonal nanoplates. Remarkably, we find that the 3D chiral Hart gyrangle can be assembled from one-component achiral triangular nanoplates decorated with regioselective complementary DNA interaction sites. In addition, Petrie-Coxeter and Hart assemblies are facetted versions of two of the simplest triply periodic minimal surfaces, namely Schwarz' Primitive and Schoen's Gyroid surfaces respectively, offering new routes to those bicontinuous nanostructures, which are widespread in synthetic and biological materials.



**Figure 2** Growth of the truncated octahedral sponge  $\{6,4,|4\}$  and the gyrangle assemblies. For the latter four colors are guides to the eye. Snapshots from simulations showing growth: (a, g)  $5 \times 10^6$ . (b, h)  $2.5 \times 10^7$ . (c, i)  $5 \times 10^7$ . (d, j)  $10^8$ . (e, k)  $2 \times 10^8$ . (f, l)  $4 \times 10^8$  (MCS).

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### Hexagulation numbers: magic numbers on the gyroid surfaces

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Regular structures of equal spheres on the gyroid minimal surfaces have been investigated as obtained through Monte Carlo simulations of hard spheres undergoing the Alder transition<sup>1,2</sup>. Remarkably, there exist magic numbers (Figure 1) producing regular structures, which are simply explained in terms of hexagulation numbers defined as  $H = h^2 + k^2 - hk$ , in with the Caspar and Klug's analogy triangulation numbers  $T = h^2 + k^2 + hk$  for icosahedral viruses, where h and k are nonnegative integers<sup>3</sup>. The total number of spheres per cubic unit cell N is represented by N = 16H. Here we extend our simulations up to H = 21. When H is a multiple of three, we find that the space group  $Ia\overline{3}d$  is broken into  $I\overline{4}3d$ ,



**Figure 1** (a) Caspar and Klug's *T*-diagram for counting the triangulation number *T* and (b) *H*-diagram for counting the hexagulation number *H*. Lattice points denoted as (h, k) with *h*, *k* nonnegative integers in two oblique coordinate systems indicate circled numbers  $T=h^{2}+k^{2}+hk$  and  $H=h^{2}+k^{2}-hk$ : *T* is half the number of lattice points inside a triangle (solid line), while *H* is the number of dashed hexagons inside a hexagon (solid line). Shown here are T=13 with (3,1) and H=7 with (3,1).

which is chiral with right- and left-handed version. These arrangements are analyzed in terms of the space groups, equivalent positions (Wyckoff positions), and polygonal-tiling representations (Figure 2). We also present bilayer regular structures composed of both right- and left-handed chiral layers having multiple of three *H* numbers.



Figure 2 Top: Regular structures of hard spheres on the gyroid surface ( $Ia\overline{3}d$ ). Bottom: their polygonal-tiling representations. H is the Hexagulation number and N is the number of spheres in a cubic unit cell. Colors indicate Wyckoff positions. Structures for H = 12 and H = 21 are chiral (I43d) having right- and lefthanded version, both of which been have obtained bv simulations.

The key is that only a limited number of efficient physical designs are possible even on negatively curved triply periodic minimal surfaces<sup>4</sup> like in icosahedral viruses. Future applications of such regular arrangements are to construct complex assemblies using the concepts of bijels, coloidosomes, polymersomes, and DNA-origami self-assemblies<sup>5</sup>.

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# Molecular understanding of mechanical properties of Archimedean tiling through star terpolymer thin film

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The eleven Archimedean tilings, suggested by Johannes Kepler [1], are described by the number of edges of polygons meeting at each vertex. These tiling patterns rarely occur naturally but can be replicated in specific synthetic polymers. The 3-miktoarm star terpolymers of different arms can form these tiling patterns based on the arm length ratio, displaying rich self-assembled morphologies [2].

This study utilized many-body dissipative particle dynamics simulations [3] with coarse-grained molecular models to investigate the relationship between morphologies and mechanical properties. Simulations were performed on single and binary systems of miktoarm star terpolymers with varying arm length ratios (Fig. 1a).

Morphology: Archimedean tiling patterns appear when the arm length ratio (x) is between 0.5 and 3.0, with broader interfaces than lamellae structures. These interfaces are widest at x = 1.0 and 1.5, corresponding to specific tiling patterns.

Mechanical Properties: Under tensile deformation, systems with broader interfaces showed more robust mechanical responses. This is due to the junctions connecting distinct domains, similar to cross-links, which resist void growth. Systems with smaller homogeneous domains exhibit less void formation, leading to improved mechanical properties.

Fracture Behaviors: Two fracture modes were identified: simple void enlargement and aggregation into larger cavities. Systems with Archimedean tiling experienced constrained void expansion, resulting in numerous small voids that eventually merged (Fig. 1b). A void-fibril network formed during deformation in binary mixtures with semi-tiling structures, preventing large cavities.

In summary, the mechanical properties of miktoarm star terpolymer thin films are closely related to the morphology, specifically the interface area. Archimedean tiling patterns offer superior mechanical properties compared to lamellae structures. The addition of different



x=5.00 (Alternating lamellae)

**Figure 1** (a) Schematic representation of coarsegrained molecular models with different arm length ratios (b) Representative snapshots of fracture behaviors at strain 120%, which is before the fracture finishes

star terpolymers can either weaken or strengthen the material, depending on the morphology changes they induce. These findings provide insights into designing polymeric materials with desired mechanical properties by controlling the molecular arrangement and morphology.

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## Understand the Relative Stability of Single-Gyroid to Double-Gyroid in AB-type Block Copolymer

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The self-assembly of block copolymers provides a versatile way for the fabrication of ordered nanostructures that have broad promising applications. One type of the most intriguing structures is the triply periodic network (TPN) structure. For many AB-type block copolymers, one TPN phase commonly appears between the cylindrical and lamellar phases in the phase sequence along increasing the composition from asymmetric to symmetric, i.e. double-gyroid (DG) <sup>[1]</sup>. The DG structure consists of two continuous tubular domains that are intercatenated throughout the slab-like matrix and are separated by the triply periodic minimal surface (TPMS). In addition to the double-network TPN structures, there are also single-network structures consisting of only one continuous network spanning throughout the matrix.

It has been commonly accepted that the bicontinuous double-gyroid (DG) network structure is the usual stable phase formed in pure AB-type block copolymer melts. Thus, the emergence of the single-network counterpart, i.e. single-gyroid (SG), is mysterious. In the previous work, it was proposed that the SG phase was stabilized by the synergistic effect of the local segregation between two unequal end B-blocks and the stretched bridging middle B<sub>2</sub>-block of linear B<sub>1</sub>AB<sub>2</sub>AB<sub>3</sub> pentablock, however, which was not sufficiently verified <sup>[2]</sup>. Here we reexamine the stabilization mechanism of the single-gyroid phase, and we reveal that the bridging middle B-blocks do not play a key role in stabilizing the SG phase over DG due to its negligibly low bridging fraction. Instead, the middle B<sub>2</sub>-blocks mainly concentrate nearby the interface in the form of loops, helping short end B<sub>1</sub>-block to push long B<sub>3</sub>-block to fill the further space and thus relieving the packing frustration of B-blocks in the matrix of SG on the one hand. On the other

hand, the middle B-block is distributed more uniformly on the interface in the SG structure than in the DG structure due to the more uniform interfacial curvature of the former. The two factors lower the relative interaction energy of SG to DG, consequently stabilizing SG. Clearly elucidating the stabilization mechanism of SG may provide guide for further improving its stability or for obtaining other single-network phases (e.g. singlediamond).



Figure 1 The stability of SG is related to the interfacial curvature and chain packing

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# Hybrid Structures Formed by Asymmetric ABC-type Block Copolymers

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Block copolymers (BCPs) provide a versatile platform for the formation of various nanostructures. Among them, ABC-type BCPs hold significant potential for creating complex structures, which have promising applications in nanotechnology. Especially when the A and C components are asymmetric, ABC-type block copolymers can form asymmetric ordered structures, or even hybrid structures of different geometric shapes composed of A and C domains. However, the self-assembly behavior of ABC-type block copolymers has not been well understood due to its complexity.

In this work, based on the ordered structures of AB-type block copolymers, we propose a useful rule to systematically assume ordered structures possibly formed by ABC-type BCPs. We then introduced topological asymmetry into the ABC system (i.e., A(BC)<sub>m</sub> miktoarm star), allowing A and C components to form domains of different shapes. By employing Self-Consistent Field Theory (SCFT), a series of novel hybrid structures, including sphere-diamond and spheres within double-gyroid networks, were predicted to be stable due to the combination of compositional and topological asymmetry. We conjecture that the balance between the stability of the A and C domains in ABC-type block copolymers is crucial for the formation of these novel hybrid structures. Our work provides a useful guide for the exploration of novel structures in ABC-type BCPs, and demonstrates that the combination of compositional and topological asymmetry can lead to the fabrication of novel hybrid morphologies.



Figure 1. Novel hybrid structures formed by asymmetric ABC-type block copolymers

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## Molecular Weight Dependence of Domain Spacing in the Double Gyroid Structure of ABC Triblock Copolymers

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Self-consistent field theory (SCFT) predicted that the region in the phase diagram of AB diblock copolymers where the double gyroid structure forms are narrow compared to other structures [1]. Experimental results agree with this prediction [2]. Therefore, confirming the double gyroid structure and the molecular weight dependence of the domain spacing in AB diblock copolymers over a broad molecular weight range is experimentally challenging.

On the other hand, in the phase diagram of a symmetric ABC triblock copolymer, also obtained with SCFT, with an equal block ratio of A and C, a double gyroid structure is predicted to form over a relatively wide range compared to the AB diblock copolymer [3]. Therefore, it is expected that the ABC triblock copolymer will be able to stably form the double gyroid structure even in the high molecular weight region compared to the AB diblock copolymer.

This study investigated the molecular weight dependence of the domain size of the double gyroid structure of poly(isoprene-b-styrene-b-2-vinylpyridine) (ISP) triblock copolymer as the ABC triblock polymer. Five samples of ISP were synthesized by living anionic polymerization, and transmission electron microscopy (TEM) and small-angle X-ray scattering (SAXS) observation were done on these samples, and SCFT simulations[4] were done for the symmetric ABA triblock copolymer with the conditions  $\chi_{AB} = 1.2$ , 1.8, and chain length  $N = 25 \sim 100$ .

The molecular weight dependence of the domain spacing is shown in Figure 1. The experimental result showed the relation

$$D = 0.108 M_{\rm n}^{0.57}$$

SCFT showed the relation  $D \propto M_n^{0.71}$  in both  $\chi_{AB} = 1.2$ ,

and 1.8, and the plots are scaled to match the point for N = 25 to Mn=65,300 in Figure 1. From this point, the experimental and SCFT results agree on the region where the molecular weight is about twice as high. However, the experimental result is lower than that of SCFT at higher molecular weights. This discrepancy is expected because the experiment was performed with an ABC structure, whereas SCFT was performed with a symmetric ABA



Figure 1 Relationship of D vs Mn

structure. A more detailed comparison will be required in the future.

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Poster P3-5 15:20-17:20, November 20 (Wed)

## Polymer Membrane Tensegrity: Inverse Design of Polymer Films Morphing into Arbitrary 3D Surfaces with Digital Photopatterning Technique

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As Goethe discussed in his seminal work, "Metamorphosis of Plants" published in 1790 [1], diverse plant morphologies, such as flowers and fruits, originate from transformed leaf-like structures. Recent studies have shown that these transformations occur through in-plane differential contraction and growth, along with the distribution of differential rigidity. Similarly, we propose a technique "Polymer Membrane Tensegrity" to fabricate arbitrary 3D surfaces from self-morphing 2D polymer films. Our technique combines polymer science and origami engineering, leveraging the expertise cultivated by our team members over the years. Fukunishi et al. have developed a method called Digital-Photopatterning using a 3D printer, where monomers embedded in the parent polymer film are selectively polymerized in specific areas, creating films with varied in-plane material properties [2]. This method thus precisely controls in-plane swelling or shrinkage in selected areas, facilitating the spontaneous formation of 3D surfaces from 2D films.

However, designing an arbitrary 3D surface still requires an inverse design approach to compute the in-plane patterns of material properties. To address this, we applied an algorithm proposed by Shimoda et al., which optimizes the locations and geometries of rigid rods on the shrinking membrane to create the desired 3D surfaces [3]. The resulting 3D surfaces are established as tensegrity structures, where the rigid rods do not connect each other but rather balance the membrane's tension to maintain the overall structural integrity. This approach enables the inverse design of 2D film patterns to achieve the intended 3D transformations [Fig.1]. We report our findings on the potential of Polymer Membrane Tensegrity in creating diverse 3D surfaces, including minimal surfaces such as Gyroid[4].



Figure 1 Fabrication process of polymer membrane tensegrity for inverse design of a target 3D surface.

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## Changes in two-dimensional small-angle X-ray scattering pattern by uniaxial stretching of a double-gyroid block copolymer

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We report an experimental observation of collapse of the Ia3d symmetry by stretching of an elastomeric block copolymer that forms a double-gyroid (DG) microdomain structure. The specimen used is polystyrene-*block*-polybutadiene-*block*-polystyrene (SBS) triblock copolymer with Mn =  $8.5 \times 10^4$ , Mw/Mn = 1.05, and  $\phi_{PS} = 0.32$  where Mn and Mwdenote the number- and weight-average molecular weights, respectively, and  $\phi_{PS}$  is the volume fraction of polystyrene (PS) blocks. A toluene solution of this sample with ca. 5 wt% of the initial polymer concentration was cast at room temperature. After complete evaporation of the solvent for about 7 days, an as-cast film obtained was then thermallyannealed at 190 °C for about 24 h to form a well-ordered DG structure. The microphase-separated structures were analyzed by using the 2D SAXS technique with synchrotron X-rays at BL-10C SAXS beamline (PF, Tsukuba, Japan) and also at BL-45XU SAXS beamline (SPring-8, Nishi-Harima, Japan).

As shown in Figure 1, the stress-strain curve exhibited strong yielding in the first-step elongation, and then the second-step elongation it exhibited some rubbery-like behavior. The strong yielding suggests that the hard PS gyroid networks underwent fracture. According to the labeled position (a)-(h), the two-dimensional small-angle X-ray scattering (2d-SAXS) patterns were measured as shown in Figure 2. Two new diffraction spots were observed for a deformed DG structure. These spots were assigned to  $\{110\}$  and  $\{200\}$  reflections ( $\sqrt{2}$  and  $\sqrt{4}$ ). For the Ia3d symmetry, these reflections are prohibited by the extinction rule and therefore none of them appeared for the specimen before deformation.

Appearance of these reflections indicates breakdown of the extinction rule and can be explained as a result of collapse of the symmetry of glide when three-dimensional DG networks are partially ruptured upon stretching [1].

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**Figure 1** Stress-strain curve for a DG specimen measured at a strain rate of 0.056 sec<sup>-1</sup>. The first run of the stretching of the virgin DG specimen is conducted up to  $\varepsilon_1 = 2.0$ . Here,  $\varepsilon_1$  designates strain for the first run of stretching, as defined by  $\varepsilon_1 = (l_0 - l)/l_0$ , with  $l_0 (= 15 \text{ mm})$  and *l* being, respectively, longitudinal lengths of the virgin and stretched films. From  $\varepsilon_1 = 2.0$ , the strain was in turn reversed until the stress reached zero. The stress recorded during this process is shown in a dotted curve. Right after this process, the second run of the stretching was performed.



**Figure 2** 2D SAXS pattern (gray-scale displays logarithm of the scattering intensity) of the through view. (a) Virgin film, (b) at  $\varepsilon_1 = 2.0$  from the virgin film, (c) relaxed from  $\varepsilon_1 = 2.0$  (no load but with residual strain  $\varepsilon_r = 0.8$ ), and (d) ~(h) restretching of the relaxed film at  $\varepsilon_2 = = 0.2$ , 0.4, 0.6, 0.8, and 1.0, respectively. The value of strain for the second run of stretching,  $\varepsilon_2$ , was defined with respect to the stretched-and-relaxed film [taking Fig. 2c at  $\varepsilon_r = 0.8$  as a reference] and hence  $\varepsilon_2 = (\varepsilon_1 - \varepsilon_r)/(\varepsilon_r + 1)$ . Except in Fig. 2a, the SD is perpendicular to the equator.

# Hierarchical Self-assembly Behaviors of ABC-Type Bottlebrush Copolymers

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Bottlebrush copolymers (BBCPs) can rapidly self-assemble into ordered nanostructures with large domain spacings, offering promising applications in nanotechnology. Recently, experiments have shown that the self-assembly of ABC-type BBCPs is an efficient method for creating hierarchical nanostructures, where the superstructure and substructure can be separately controlled by varying the number or lengths of the side chains. However, the self-assembly behaviors of ABC-type BBCPs are influenced not only by the volume fraction but also by the side chain asymmetry and the rigidity of the backbone, making them complex and therefore not well understood. In order to explore more hierarchical structures and fully understand the self-assembly behavior of ABC-type BBCPs, systematic studies are needed.

In this work, we have performed dissipative particle dynamics simulations to study the self-assembly of ABC-type BBCPs. One portion of the backbone is grafted with pairs of A-blocks, while the other portion is grafted with pairs of B/C-blocks. Our focus is on the effects of the grafting number of A side chains, the length of B side chains relative to C side chains, and the rigidity of the backbone on the formation of hierarchical structures. We observed a multitude of hierarchical structures where the superstructures are formed by the phase separation between A and B/C blocks, and the substructures are formed by the phase separation between A and B/C blocks, and the substructures are formed by the phase separation between B and C blocks. Although the formation of A-superstructures and B-substructures in many hierarchical structures can be independently controlled, there are also hierarchical structures where the transitions of the superstructure and substructures are coupled. Additionally, our results reveal that a rigid backbone favors the normal arrangement of B-substructures relative to A-superstructures. Our work not only deepens the understanding of the self-assembly mechanisms of ABC-type BBCPs but also introduces new design principles for the efficient creation of complex hierarchical structures.



Figure 1 Schematic of the self-assembly behaviors of ABC-type bottlebrush copolymers.

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#### Gyroid Interface from Symmetric ABCD Tetrablock Quarterpolymers by Monte Carlo Simulation

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ABC triblock terpolymers consisted of three incompatible polymer chains naturally form three-phase structures in bulk state. Morphologies of the molecules whose volume fraction of A-chain is equal to that of C-chain,  $\varphi_A = \varphi_C$ , have been well studied, where they possess two interfaces, A/B and B/C, which do not intersect each other because the A- and C-phases are pulled apart by the B-chains. The symmetric terpolymers show the tricontinuous gyroid structure around  $\varphi_B = 0.5$  [1,2]. The two interfaces, A/B and B/C, are different from the Schoen's gyroid surface, because  $\varphi_A$  and  $\varphi_C$  are much smaller than 1/2, while the trajectory of the center of the B-chains can be statistically described as the gyroid surface. The visible A/B and B/C interfaces are a pair of level surfaces derived from the Schoen's gyroid. Triply periodic minimal (TPM) surfaces including gyroid have not been observed as interfaces of microphase-separated structures in block polymer systems so far, and interfaces with zero mean curvature formed by block copolymers have only been observed in lamellar phase, which can be simply recognized as a flat surface. In this study we try to obtain and visualize TPM "interface" in phase structures of symmetric ABCD tetrablock quarterpolymers where the two conditions with respect to volume fractions,  $\varphi_A = \varphi_D$  and  $\varphi_B = \varphi_C$ , hold, while a volume fraction parameter,  $\varphi = \varphi_C + \varphi_B$ , as the sum of B- and C-phases, is defined.

At first, we simulated the stable structure in the medium  $\varphi$  region, and obtained the lamellar structure whose repeating unit is ABCDCB in the range of  $\varphi < 0.625$ . A phase transition from the lamellar to tetracontinuous structures is observed at  $\varphi=0.625$  with increasing  $\varphi$ . This newly found structure is stable for certain  $\varphi$  region, but finally another



**Figure 1** The shape and distributions of mean curvature H on the (a) A/B and (b) B/C interfaces using the color scale [3].

lamellar structure appears at  $\varphi$ =0.8125. The composition range of the tetacontinuous structure has been found to be 0.625  $\leq \varphi \leq 0.75$ , and the three-dimensional surfaces of A/B and B/C interfaces are shown in Figure 1. It is found that the A/B interface is equivalent to the C/D interface and the A/B and C/D interfaces can be regarded as the level surfaces to the gyroid surface. The B/C interface divide into two subspaces with equal volume. Figure 1 compares the distribution of mean curvature *H* on the interfaces using the color scale. The averaged *H* values with their standard deviations are  $\langle H_{AB} \rangle = 1.08 \times 10^{-1} \pm 0.110$ and  $\langle H_{BC} \rangle = 4.39 \times 10^{-4} \pm 0.0307$ , indicating that the mean curvature of the B/C interface, where the centers of polymer chains stay on, is nearly zero, and hence we conclude the visible interface can be described as the Schoen's gyroid surface.

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## Interfacial Segment Distribution of a Diblock Copolymer in a Polymer Thin Film

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The composite polymer material forms various morphologies of phase-separated structure with interface between the different phases. The interfacial width between the phases is one of important factors for enhancing mechanical strength of the composite material or adhesion strength. Neutron reflectometry is an indispensable technique for structural analysis on a surface, an interface, and a thin film with a high spatial resolution of sub-nm scale in a non-destructive manner. So far, the interfacial segregation of the component has been clarified for the polymer blend thin films with the different molecular weights or the different tacticity by using neutron reflectometry [1, 2]. In this study, the interfacial segment distribution of a diblock copolymer in a polymer thin film was investigated by neutron reflectometry with a deuterium labeling method.

A diblock copolymer of deuterated styrene and 2-vinylpyridine with the molecular weight of  $44\times10^3$ and  $17\times10^3$ , respectively, was used. The poly(2-vinylpyridine) (P2VP) has strong affinity to the hydrophilic surface of a silicon substrate. The blend thin films of hydrogenous polystyrene (hPS) with the molecular weight of  $10\times10^3$  or  $51\times10^3$  and the diblock copolymer were prepared by spin-coating from the dilute solution of chloroform or toluene, which is a common good solvent or selective solvent for polystyrene, respectively. Neutron reflectivity (NR) measurement was conducted on the SOFIA neutron reflectometer [3] at the BzL16, Materials and Life Science Experimental Facility (MLF), Japan Proton Accelerator Research Complex (J-PARC), Tokai, Ibaraki, Japan. The depth scattering length density (SLD) profile was obtained by a conventional model analysis on the specular reflectivity data.

The as-prepared blend thin films exhibited the interfacial segregation of the diblock copolymer, and its segregation was more enhanced by thermal annealing. The interfacial segregation of the block copolymer was more pronounced in the hPS with the higher molecular weight. Figure 1 compares the depth SLD profile for the hPS thin films with the diblock copolymer, spin-coated from the solution in toluene or chloroform. It was found that the diblock copolymer having the higher SLD segregates at the interface with the silicon substrate, because the SLD profile exhibited the higher value near the interface. Moreover, the block copolymer more segregated at the interface in the hPS thin film prepared from toluene than from chloroform due to the difference in solvency for the component.



Figure 1 The SLD profile as a function of distance from the interface for the PS thin films with the diblock copolymer spin-coated from the solution in toluene or chloroform.

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#### Hierarchical gyroid structures in frustrated ABC triblock copolymers

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Frustrated linear ABC triblock copolymer with the repulsive interaction between A and C blocks significantly weaker than those between the other two pairs of adjacent blocks can self-assemble into various hierarchical structures composed of discrete B-subdomains sitting on A/C interfaces. However, whether the hierarchical structures still follow the common transition sequence of sphere  $\rightarrow$  cylinder  $\rightarrow$  gyroid  $\rightarrow$  lamella remains an interesting question to be answered. In this work, the self-assembly of frustrated linear ABC triblock copolymer is investigated using self-consistent field theory (SCFT), focusing on the formation of different hierarchical gyroid structures.

Since these hierarchical gyroid nanostructures may be used to fabricate functional materials with high performance, it is critical to choose the A, B and C monomers for obtaining three proper Flory-Huggins parameters based on the phase diagram. Specifically, we consider that short middle B-blocks form discrete subdomains decorated on the surface of A-domain. We first construct the corresponding part of the triangular phase diagram with respect to three compositions ( $f_A$ ,  $f_B$  and  $f_C$ ) for fixed  $\chi_{AB}N = \chi_{BC}N = 80 \gg \chi_{AC}N = 15$ . Surprisingly, the hierarchical gyroid structure is not commonly formed between the hierarchical cylindrical and lamellar structures in the transition

sequence with changing  $f_A$ . For these hierarchical structures, the formation of B-subdomains on the surfaces of A-domains presents a constraint on the chain configurations, leading to entropy loss. Accordingly, we speculate that the absence of the gyroid structure is mainly caused by its irregular surface of A-domain that does not allow the B-subdomain to form uniform arrangement and thus produces more severe constraint on the chain configurations than the cylindrical and lamellar structures with regular surfaces of A-domains.



The stability regions of various gyroid phases appear and expand as  $\chi_{AB}N$  is gradually decreased, giving rise to the common transformation from cylinder to gyroid and then to lamella for A-domain. This is because as  $\chi_{AB}N$  decreases, the A/B interface widens and B-subdomains move into main A-domain, relieving the constraint on the A/B junction point and thus on the configuration of A-block. This work demonstrates that the substructure of the hierarchical structures imposes a nontrivial effect on the relative stability of various hierarchical structures, which may disrupt the common transition sequence in frustrated linear ABC triblock copolymer.

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Poster P3-11 15:20-17:20, November 20 (Wed)

#### Stage-wise Pre-assembly in Melt Prior to Liquid Crystals

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We investigate two unusual phenomena in self-assembly of anisotropic molecules from isotropic (Iso) melt: a heat-capacity ( $C_p$ ) maximum, and spontaneous formation of the recently discovered chiral liquid phase in achiral compounds (Iso\*). Based on experiments on newly synthesised non-chiral monomers, dimers and polymers, we construct a thermodynamic theory that shows why many liquid crystals (LC) and some crystals form in two stages, i.e. (i) continuous equilibrium growth of nano-clusters in the melt through strong intermolecular core-core interactions, causing the  $C_p$ -maximum, followed by (ii) establishment of chiral long-range order (LRO) through a second-order Iso-Iso\* transition and/or a first-order phase transition to a phase with positional LRO (Iso-LC, Iso\*-LC, Iso\*-crystal or Iso-crystal). The first process (i) is equivalent to cluster formation in solutions, known as "supramolecular polymerization", where the lack of inter-cluster interaction rules out the establishment of LRO. Furthermore, we argue that separation into a broad and a sharp transition is universal in condensed matter where strong interactions by themselves cannot lead to LRO, either because the clusters are 1D or due to strong frustration. Clusters must first grow to critical size when, at  $T_c$ , the weak interactions reach ~k<sub>B</sub> $T_c$  per cluster, prompting LRO formation. A situation similar to that in LCs is seen in spin ordering in magnetic crystals, but only near 0 K.



Figure 1. Pre-assembly of polycatenar compounds in the melt on cooling leads to increase in the correlation length (SAXS, left) and eventually the establishment of long range order. The pre-assembly is accompanied by a  $C_p$ -hump in the melt (right), which contains the majority of the enthalpy of self-assembly. This is followed by a 2<sup>nd</sup> order transition to chiral melt, before the 1<sup>st</sup> order transition to cubic or other LCs on cooling.

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Poster P4-1 15:20-17:20, November 20 (Wed)

### Structures made by termites and spiders

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Many organisms in nature construct intriguing shapes. Humans have long drawn inspiration from these natural structures, applying them to engineering fields such as architecture [1]. The structures built by organisms themselves are remarkably intricate, with many of their shapes and formation processes remaining a mystery. This study delves into the unique curved surfaces found in fungus gardens of fungus-farming termites and funnel webs of spiders; a topic that has not been extensively explored. The primary goal of this study is to unravel the morphological characteristics of these structures and to uncover potential engineering applications.

First, fungus gardens composed of specialized termite feces have porous structures. The surface of the fungus garden in the termite mound is covered with numerous mycelial pellets of *Termitomyces*, which are 2-3 mm in size. The three primary roles of the fungus garden are a source of nitrogen as preserved foods, an external digestive system to facilitate cellulose breakdown and a cellulase source. In addition, the fungus garden increases CO<sub>2</sub> levels to stabilize the mound's temperature and humidity using the mound's ventilating system [2]. In this study, the fungus garden of *Macrotermes gilvus* was observed using a computed tomography scanning model using the inspeXio SMX-225CT FPD Plus, as shown in Figure 1. The red line shown in Figure 1 is the cross-section of the scanned STL model when cut in a particular plane. The authors collected the specimen at the Sakaerat Environmental Research Station in Thailand. The shape of the fungus garden differs for each species of fungus-farming termites, and they were CT-scanned for each of them. This observation shows that the surface has a complex curve, and the cross-section confirms that the structure is internally branched and hierarchically connected.

Second, spiders in the family *Agelenidae* create funnel-webs, as shown in Figure 2. Many studies have been conducted on the shape of spiderwebs, and most of them are orb webs composed of twodimensional radial and spiral threads; however, only approximately 10% of all spiders create orb webs. Some studies have applied the Spider Web Scan (SWS) laser-supported tomographic method to develop an experimental technique that directly measured the three-dimensional sheet-web shape using a laser and reconstructed a digital 3D model [2]. This study focuses on the formation process of the funnel-web created by *Agelenidae* to understand the curved surface's characteristics based on geometric formation factors.



funnel-web

Figure 1 STL model of fungus comb using CT scan.

Figure 2 Spiderweb of Agelena sylvatica.

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# Order and disorder of the microstructures of the *Cidaris rugosa* sea urchin stereom

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The sponge-like biomineralised calcite materials found in echinoderm skeletons are of interest in terms of both structure formation and biological function. Despite their crystalline atomic structure, they exhibit curved interfaces that have been related to known triply-periodic minimal surfaces. Here, we investigate the endoskeleton of the sea urchin *Cidaris rugosa* that has long been known to form a microstructure related to the Primitive surface (ref. 1). Using X-ray tomography, we find that the

endoskeleton is organised as a composite material consisting of domains of bicontinuous microstructures with different structural properties (ref. 2). We describe, for the first time, the co-occurrence of ordered Primitive and Diamond structures and of a disordered structure within a single skeletal plate. A representative Diamond volume is shown in Figure 1. We show that these structures can be distinguished by structural properties including solid volume fraction, trabeculae width, and to a lesser extent, interface area and mean curvature. In doing so, we



**Figure 1** A representative subvolume of the stereom that closely resembles a single Diamond surface. (A) Cross-section through the interambulacral plate showing the location of the representative subvolume. Scale bar = 1 mm. (B) The subvolume of the sea urchin stereom (in grey; isotropic voxel size of 732 nm) and a simulated nodal approximation of a single Diamond surface with a solid volume fraction  $\phi = 0.3$  (in yellow).

present a robust method that extracts interface areas and curvature integrals from voxelized datasets using the Steiner polynomial for parallel body volumes. We discuss these very large scale bicontinuous structures in the context of their function, formation, and evolution.

This work was supported by the Australian Research Council (ARC) through the Discovery Project DP200102593. A.J.M is supported by an Australian Government Research Training Program (RTP) Scholarship.

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#### Chirality of gyroid-type photonic crystals in the scale of *Teinopalpus Imeperialis*

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The intricate nanostructures responsible for vivid structural colors in certain insects have attracted attention. The wing scales of butterflies and the scales of beetles are known to possess photonic crystals based on mathematically defined minimal surfaces. While many weevils have diamond-type minimal-surface-based photonic crystals within their scales, some butterflies, such as *Callophrys rubi*, have gyroid-type minimal-surface-based photonic crystals. These nanostructures exhibit vivid colors known as structural colors due to their periodicity, and research on their optical properties and applications in materials science has been intensively conducted.

However, how organisms form such complex structures remains a challenging question. Gyroidtype photonic crystals are chiral, and thus have left-handed (LH) or right-handed (RH) helical structures, depending on which of the two spaces separated by the minimal surface is filled with cuticle. It has been reported that LH gyroid-type photonic crystals in the scales of *Callophrys rubi* are found to be more frequent than RH gyroid-type photonic crystals[1]. Another butterfly (*Thecla opisena*) with gyroid-type photonic crystals inside its scales is similarly indicated to have more LH gyroid-type photonic crystals than RH ones[2]. This suggests that when the butterfly forms gyroid-type photonic crystals, the direction in which the cuticle is filled is unbalanced. The chiral imbalance provides valuable insights into the formation mechanism of the gyroid structure.

In this study, we investigate the chirality of the gyroid-type photonic crystal in another butterfly (Teinopalpus Imeperialis), which possesses gyroid-type photonic crystals. The distinctive green coloration of Teinopalpus Imeperialis, as shown in Figure 1(a), originates from the periodic network structure inside the scales, which are known to be gyroid-type photonic crystals (Figure 1(b)). The crystals inside the scales are polycrystalline and are composed of microcrystals that are called domains, which are assembled without gaps between them. A recent previous study using small-angle X-ray scattering has revealed that the scales on the dorsal side have the [111] direction of the gyroid structure facing the scale surface [3]. The [111] direction of the gyroid structure has through holes and is comparatively easy to distinguish the orientation of the helix. Thus, we prepared the frontal section of the scale and observed the section of the nanostructure. We report the results of our investigation of the chirality of the gyroid structures.



**Figure 1:** (a) Photograph of *Teinopalpus Imeperialis* and micrograph of a green scale. (b) Electron micrograph of a cross-section of the scale. The inset shows a schematic diagram of a gyroid-type photonic crystal.

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Poster P5-1 15:20-17:20, November 20 (Wed)

### Non-Fourier Computations of Heat and Mass Transport in Nanoscale Solid-Fluid Interactions Using the Galerkin Finite Element Method

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This study investigates the enhancement of thermal performance in base fluids through the dispersion of three types of nanoparticles, utilizing a novel non-Fourier heat transfer theory. The focus is on comparing the thermal efficiencies of various nanoparticle and nanogyroids combinations to determine the optimal configuration for improved fluid thermal performance. Employing the Galerkin Finite Element Method (GFEM), the research delves into how the nanoparticles influence thermal dynamics, with models developed based on non-Fourier heat flux theory, computational fluid dynamics (CFD) conservation laws, and no-slip thermal boundary conditions. The numerical solutions, validated against published data, involve grid-sensitivity tests and assessments of solution accuracy, correction, and stability, examining critical parameters like wall shear stress, mass flow rate, and heat flux in relation to rheological variables and thermal relaxation time.

The findings highlight the significant role of thermal relaxation time—the duration a fluid takes to return to thermal equilibrium—in influencing fluid temperature. Simulations indicate that mono nanofluids exhibit the most pronounced impact on fluid temperature due to having the longest thermal relaxation times, whereas ternary nanofluids display the shortest. Moreover, ternary nanofluids show a greater thermal boundary thickness compared to mono and binary nanofluids, and the highest values of wall heat and mass flux are observed in non-Fourier scenarios of heat and mass diffusion, suggesting a superior thermal performance over traditional Fourier methods. These insights pave the way for optimized nanoparticle and nanogryroids enhanced thermal fluids, offering substantial improvements in thermal management technologies.

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# Heat enhancement using Gyroid Structure and metal foam for **Different Porosity and Cooling fluids: Experimental and Numerical Approaches**

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Porous media has been used in engineering applications for many years. The advantage of such material is its lightweight and efficient cooling process. Metal foam is one class of porous material and is produced by industry. Thus, the user is limited by the available porosity, permeability, and design. Designing a new class of material using triply periodic minimal surfaces has been available for a long time. This mathematical formulation is currently used to create different structures suitable for the thermo-fluids discipline, material discipline, and biomedical field.

Various researchers in the field of engineering have used porous media for many years. The present paper studies heat enhancement using two different types of porous media. In the first type, porous metal foam media was used experimentally and numerically for heat extraction. The porous medium was replaced with a porous structure using the Gyroid model and the triply periodic minimum surfaces technique in the second type. The Darcy-Brinkman model combined with the energy equation was used for the first type, whereas Navier–Stokes equations with the energy equation were implemented for the second type. The uniqueness of this approach was that it treated the Gyroid as a solid structure in the model. The two types were tested for different heat fluxes and different flow rates [1,2]. A comparison between the experimental measurements and the numerical solution provided a good agreement. By comparing the performance of the two types of structure, the Gyroid structure outperformed the metal foam for heat extraction and uniformity of the temperature distribution. Despite an 18% increase in the pressure drop in the presence of the Gyroid structure, the performance evaluation criteria for the Gyroid are more significant when compared to metal foam. Figure 1 presents the gyroid with a porosity of 0.7 in the test section. Results revealed that;

1. For the metal foam, it is found that the temperature distribution along the flow is increasing toward a non-uniform cooling.

2. For the metal foam, a thermal boundary is developed along the flow, and means of breaking this thermal boundary layer must be addressed

3. Uniform temperature distribution is achieved experimentally and numerically for the Gyroid structure. The structure design allowed the break of the thermal

boundary layer. 4. The pressure drop in the metal foam appears to be less than the pressure drop in the Gyroid by an average of 18%

5. Comparing the performance of the two structures for identical conditions shows that the Nusselt number is higher for the Gyroid structure. This led to the belief that lower temperatures were achieved and a better cooling process was needed.

This work was supported by National Science and Engineering Research Council Canada (NSERC)

Figure 1 Experimental

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## **Coupling Additive Manufacturing with Triply Periodic Minimal Surface Enable Next-Generation Aero-Engine Heat Exchangers**

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The aero-engine, characterized as a highly complex and advanced thermodynamic machinery, experience a heightened thermal load on its on-board heat exchangers due to the elevating pre-turbine temperature and thrust-to-weight ratio. Triply periodic minimal surfaces (TPMS) are regarded as holding potential for constructing the next-generation heat exchangers.

Since 2021, our research group<sup>[1]</sup> has been actively engaged in exploring the applicability of TPMS as configurations for on-board heat exchangers in aero-engines, specifically focusing on fuel cooling oil cooler (FCOC). This study presents a comprehensive exploration of the TPMS-HX, covering multiple perspectives including design, manufacturing, experiment, simulation, and post-processing.

TPMS is a collection of mathematically defined surfaces that exhibit local area minimization and extend periodically in three-dimensional space. TPMS structure could effectively partitions the three-dimensional space into two interconnected yet separate domains. Among the TPMS family, the Gyroid structure is the most renowned and widely acknowledged for its suitability in constructing heat exchangers. The experimental prototype investigated in this study consisted of Gyroid structures, with a unit cell size of 4 mm and a uniform wall thickness of 0.5 mm. The prototype was manufactured using stainless steel 316L via a selective laser melting process.

Surface roughness poses a significant challenge in the application of AM-ed heat exchangers. The experimentally measured  $\Delta P_c$  surpasses the theoretical performance by 69.82% for  $\dot{m}$ =500 kg/h. The experimentally measured  $\dot{Q}_{ave}$  consistently exceeds the numerical results, with this advantage progressively magnifying as  $Re_c$  increases. Notably, the largest relative deviation occurs at  $Re_c$  of approximately 1350, reaching 8.52%.

To address this issue, this study employed abrasive jet polishing technique to finish the internal surface of the prototype. The samples were characterized using an Olympus DSX-1000. Prior to polishing, the internal surface exhibited uneven distribution with rough raised microstructures ranging from 20 to 200  $\mu$ m in diameter. These structures were attributed to partially melted metal powders adhering to the internal surface. Following the polishing process, there was a noticeable reduction in the density of microstructures, this outcome signifies a substantial decrease in surface roughness.

The *PEC* (performance evaluation criteria) value represents the comprehensive performance of studied prototype. At *Re* of 300, the pre-polishing sample exhibits an 8.08% higher *PEC* compared to the baseline. However, at *Re* of 3000, this prototype demonstrates a 12.10% lower *PEC* than the baseline, indicating no comprehensive performance advantage at high *Re*. Remarkably, after the polishing process, the Gyroid configuration consistently outperforms the baseline by 12.94% to 26.09% across *Re* range of 300-3000.

The findings and insights obtained from this work will serve as a valuable guidance and references for the development and implementation of TPMS-HX in next-generation aero-engine.

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### Sound Insulation Properties of Gyroids at Normal Incidence

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Gyroid is a bandgap structure that reflects and scatters specific wavelengths. This characteristic is responsible for the vibrant structural colors found in some kind of butterfly wing scales<sup>[1]</sup>. The objective of this study is to utilize the acoustic analogy of such photonic bandgap for sound insulation.

In this study, we focused on the sound insulation characteristics of a gyroid partition model with equal volume as a basic investigation. The model is described by:

$$-n < \sin 2\pi Ax \cos 2\pi y + \sin 2\pi y \cos 2\pi z + \sin 2\pi z \cos 2\pi Ax < n, \tag{1}$$

where parameter *n* determines the porosity. *A* decides the compression ratio along x-axis. Figure 1(a) is Normal Gyroid (A = 1), and Figure 1(b) is Compressed Gyroid (A = 2). Both has the same porosity 50% (n = 0.77).

The insertion loss of these models at normal incidence were calculated using the frequency domain finite element method. The periodic boundary conditions were applied in the y and z-axis directions, assuming a sound insulation wall with a thickness of 100 mm.

The numerical results are shown in Figure 2. The results indicate that both shapes exhibit high sound insulation performance for bandgap frequencies. To investigate the cause of this phenomenon, we discuss the elevation shape of the incident surface. Similar to perforated plates, there are evenly spaced holes, and its spacing matches the wavelength of the bandgap frequency. The periodicity of the elevation shape of the incident surface forms peaks or modes at the corresponding frequency because of Wood's anomaly<sup>[2]</sup>. This affects the bandgap of normal and Compressed Gyroid in common. Additionally, despite both having the same thickness, Compressed Gyroid in Figure 1(b) demonstrates improved sound insulation performance. This is because, Compressed Gyroid contains two periods in the incident direction, resulting in a higher sound insulation effect due to Wood's anomaly.

Based on these results, it is suggested that gyroids can lead to the development of effective sound insulation materials.



(a) Normal Gyroid

(b)Compressed Gyroid

Figure 1: Two types of Gyroid models with a side length of 100 mm.

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Figure 2: Insertion losses of Normal and Compressed Gyroids.

# From Cubic Membranes to Plasmalogen Nanomaterials: Unraveling the Role in Cell Survival, Aging, and Neurodegenerative Disorders

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Lipids may self-assemble into dynamic and complex membrane architectures ranging from simple, double, and multiple bilayer networks depicted by 3-dimensional periodic level surfaces termed "Cubic Membranes (CM)". The membrane structural dynamics is central to the diversity of roles they play in biological system, and cell membrane homeostasis might be the missing link in aging and age-related ailments, especially multiple inflammation-mediated neurodegenerative disorders. Here we introduce CM followed by CM-derived phospholipids – specifically plasmalogens (Pls), their shared properties together with CM as antioxidant and potentially anti-inflammatory function with implications in cell survival and organismal longevity [1]. We further discuss the observations of lowered levels of Pls measured across different neurodegenerative and metabolic disorders, as well as a potential strategy of restoring Pls levels via Pls replacement therapy to relieve illness and recover membrane architecture and homeostasis, and eventually promote human health. Two selected cell models with gyroid-CM mitochondria in: (1) cone photoreceptor of small mammals treeshrew (*Tupaia belangeri*), and (2) free-living giant amoeba (*Chaos carolinense*) will be presented. The advantages of plasmalogen-based self-assembled lipid nanomaterials (Fig. 1) and biomimetic nanotechnology inspired by cubic membranes will also be discussed [2,3].



**Figure 1** Liquid crystalline lipid nanoparticles (cubosomes) derived from self-assembled lipid cubic membrane phases. (Left) Plasmalogen-based cubosomes obtained by dispersion of a mixed amphiphilic mixture. (Right) Nanodomains with modified structural order induced by encapsulated drug molecules in the cubosome nanocarriers.

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