MSRI
Mathematical Sciences Research Institute

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NOTETAKER CHECKLIST FORM

(Complete one for each talk.)

Name: Malgorzata Marciniak **Email/Phone:** mmarciniak@lagcc.cuny.edu 5734620411

Speaker's Name: Jacob Kirkensgaard

Talk Title: Soft matter as a playground for the exploration of space partitioning

Date: 10 / 04 / 2018 **Time:** 3 : 30 am / pm (circle one)

Please summarize the lecture in 5 or fewer sentences:
Experimental and theoretical work on various molecules that self-assemble. Single block copolymers may have segments of cylindrical or conical shape that create supramolecular assembly and later a multigeometry assembly with given properties. Various AB deblock or ABC triblock copolymers effects of molecular architecture. With examples from biology: Cubic-lamellar transition in plant membranes, butterflies and weevils.

CHECK LIST

(This is **NOT** optional, we will **not pay** for **incomplete** forms)

☑ Introduce yourself to the speaker prior to the talk. Tell them that you will be the note taker, and that you will need to make copies of their notes and materials, if any.

☑ Obtain ALL presentation materials from speaker. This can be done before the talk is to begin or after the talk; please make arrangements with the speaker as to when you can do this. You may scan and send materials as a .pdf to yourself using the scanner on the 3rd floor.

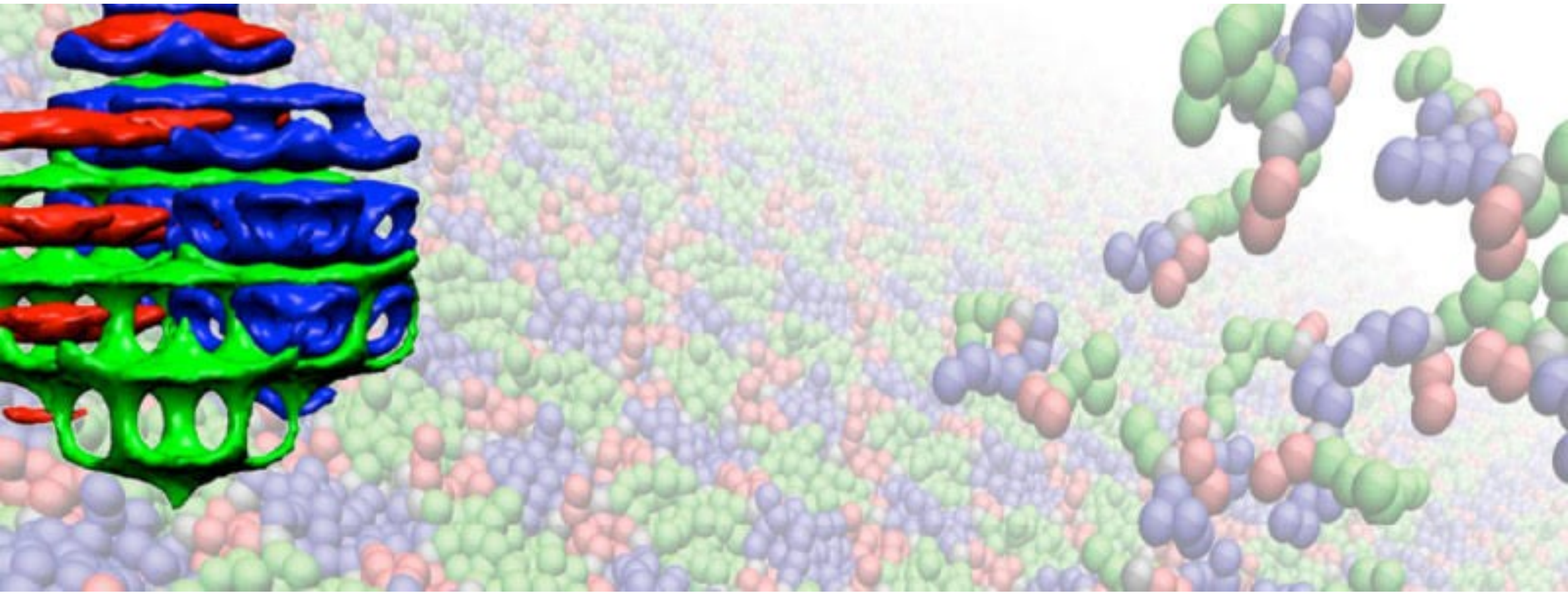
- **Computer Presentations**: Obtain a copy of their presentation
- **Overhead**: Obtain a copy or use the originals and scan them
- **Blackboard**: Take blackboard notes in black or blue **PEN**. We will **NOT** accept notes in pencil or in colored ink other than black or blue.
- **Handouts**: Obtain copies of and scan all handouts

☑ For each talk, all materials must be saved in a single .pdf and named according to the naming convention on the "Materials Received" check list. To do this, compile all materials for a specific talk into one stack with this completed sheet on top and insert face up into the tray on the top of the scanner. Proceed to scan and email the file to yourself. Do this for the materials from each talk.

☑ When you have emailed all files to yourself, please save and re-name each file according to the naming convention listed below the talk title on the "Materials Received" check list. (*YYYY.MM.DD.TIME.SpeakerLastName*)

☑ Email the re-named files to notes@msri.org with the workshop name and your name in the subject line.

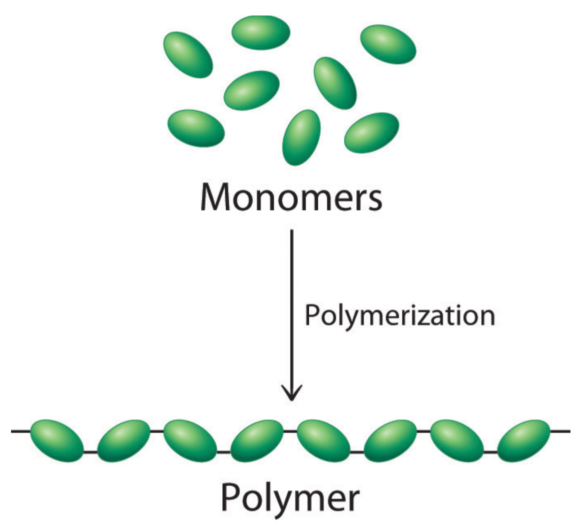
Soft matter as a playground for the exploration of space partitioning



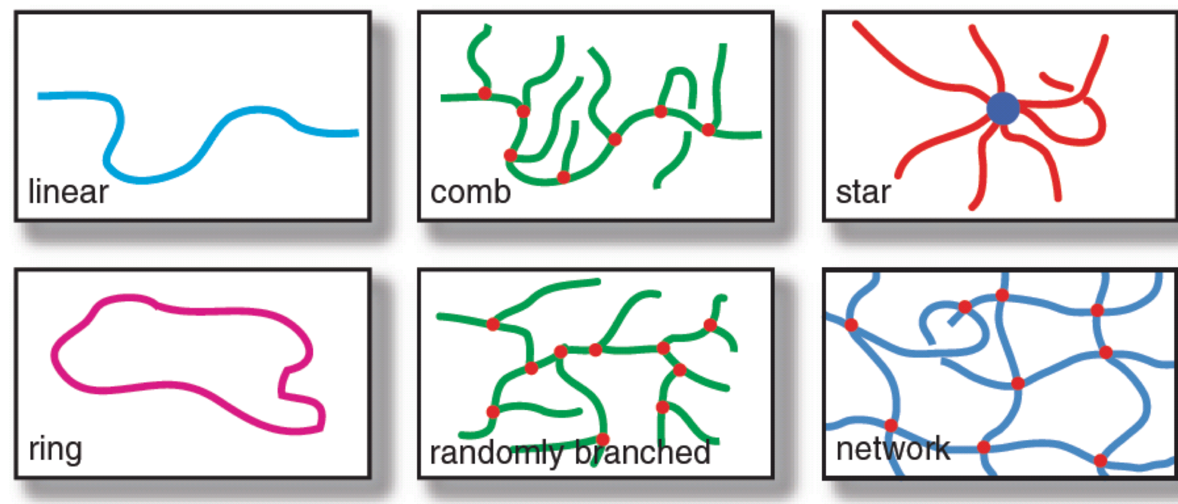
Jacob Kirkensgaard, University of Copenhagen
Hot Topics: Shape and Structure of Materials

Molecular overview

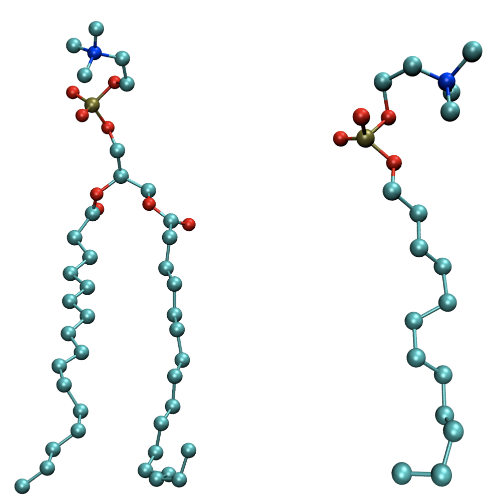
Polymers



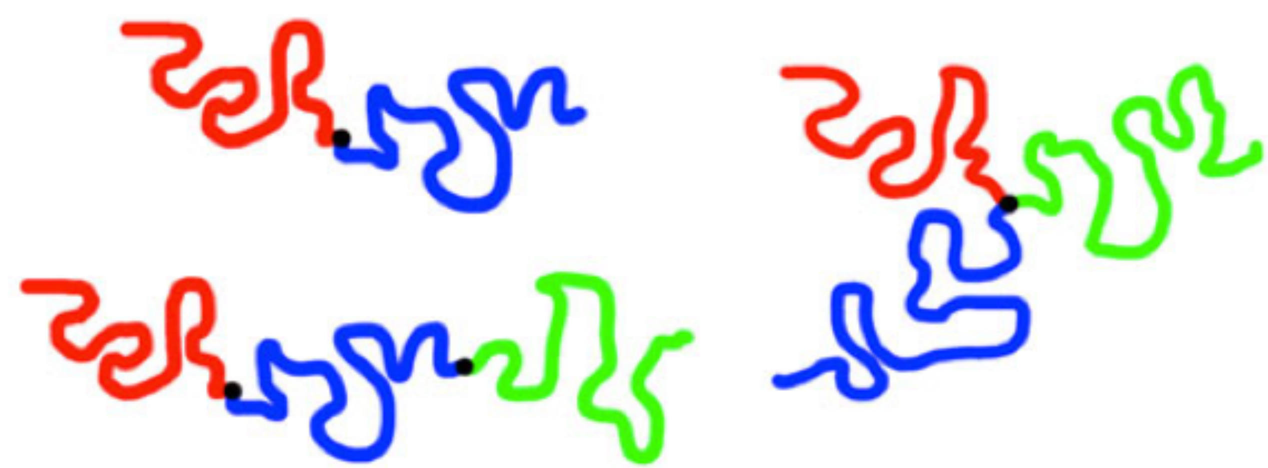
Polymer architectures



Lipids and surfactants

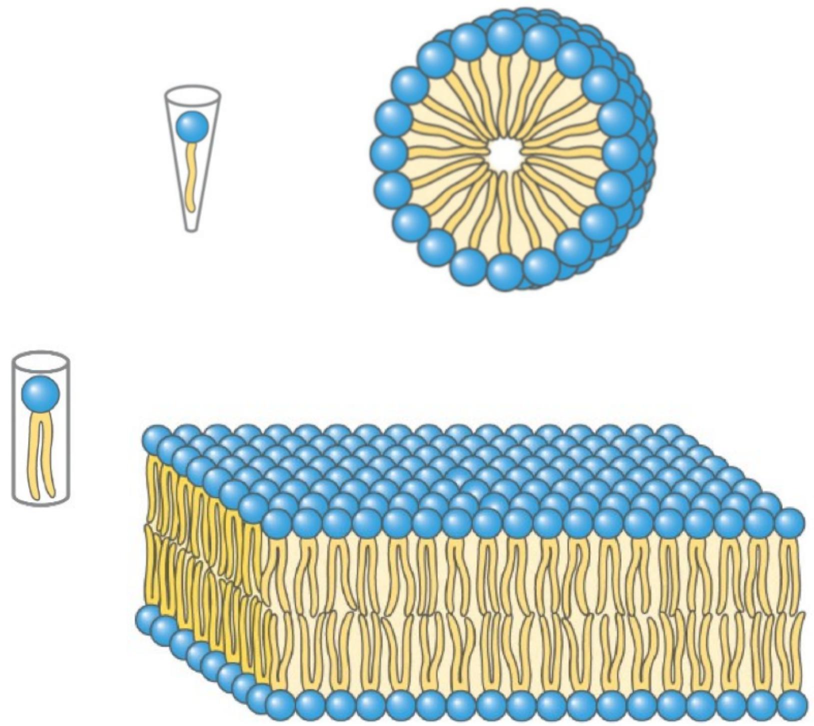


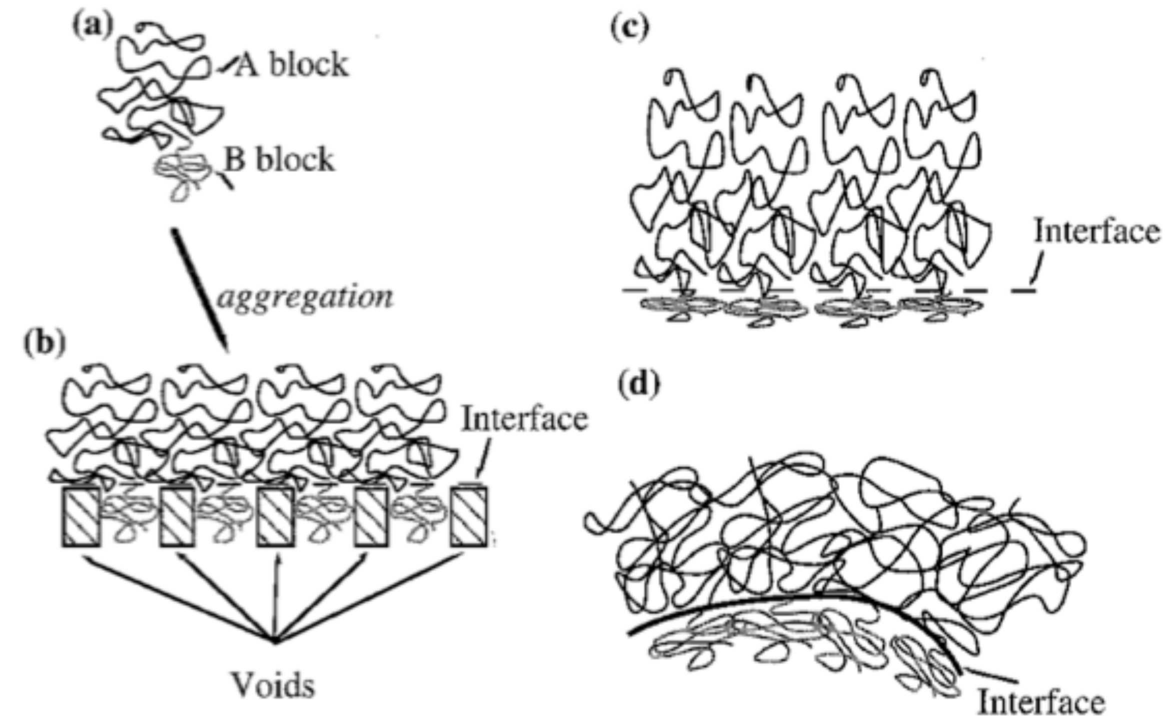
Block copolymers



In solvent or in melt state

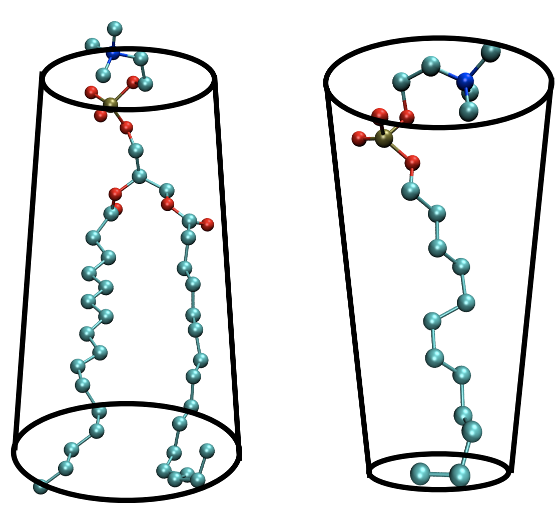
Molecular shape/geometry

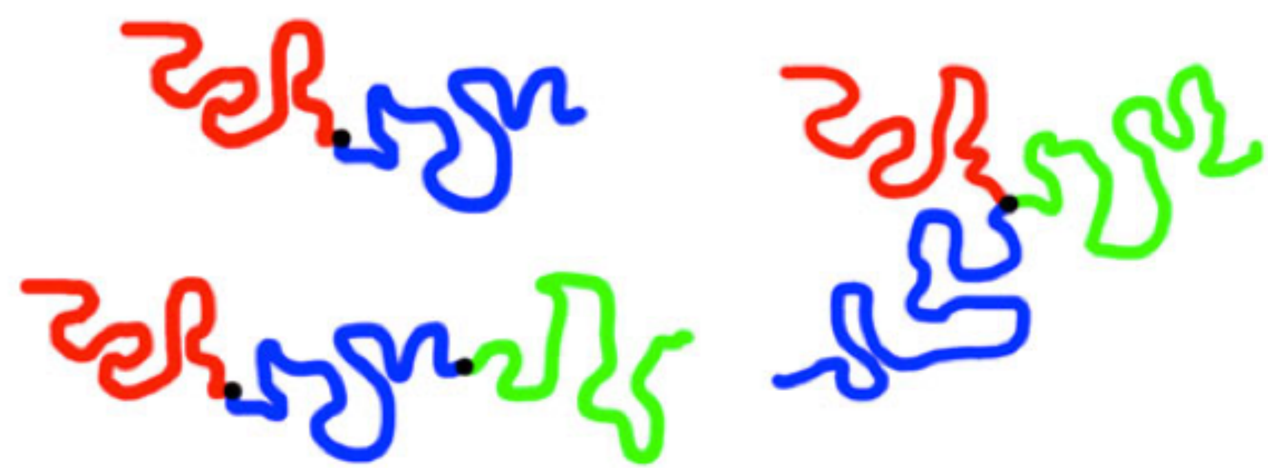




Lipids and surfactants

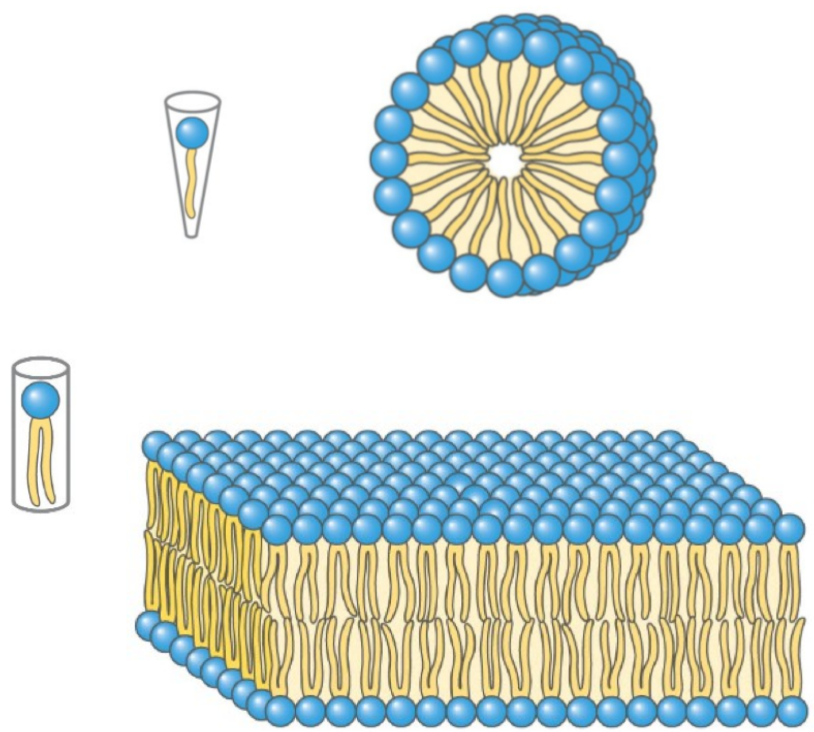
Block copolymers

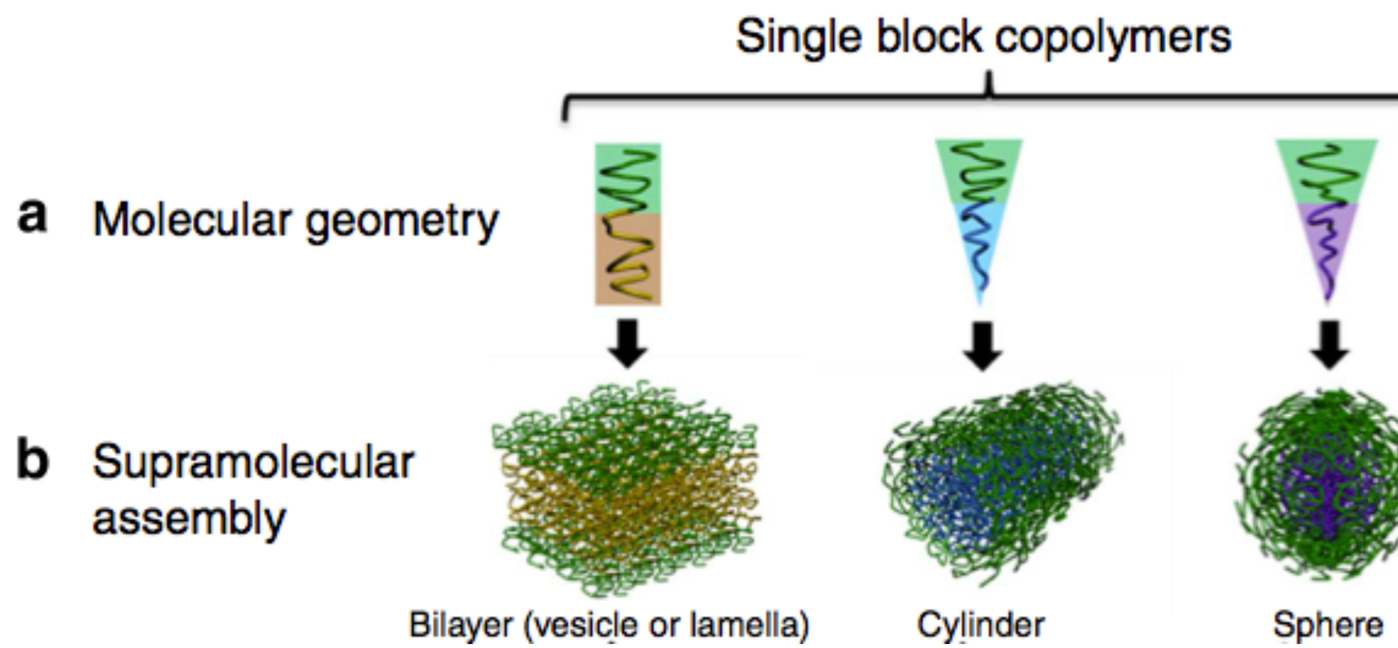




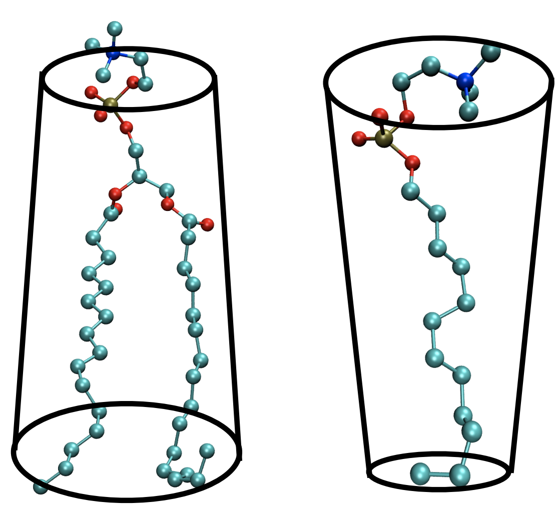
In solvent or in melt state

Molecular shape/geometry

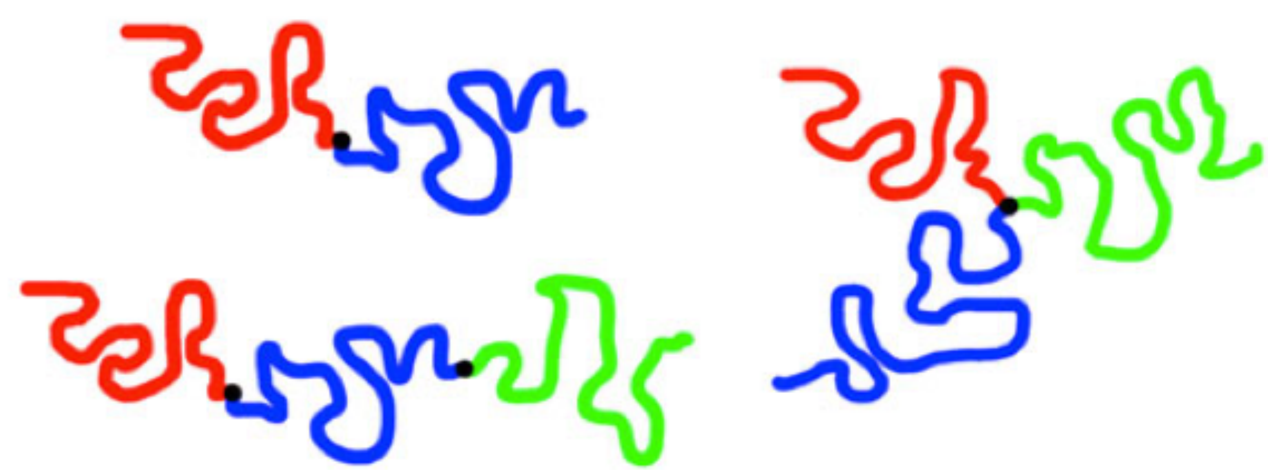




Lipids and surfactants

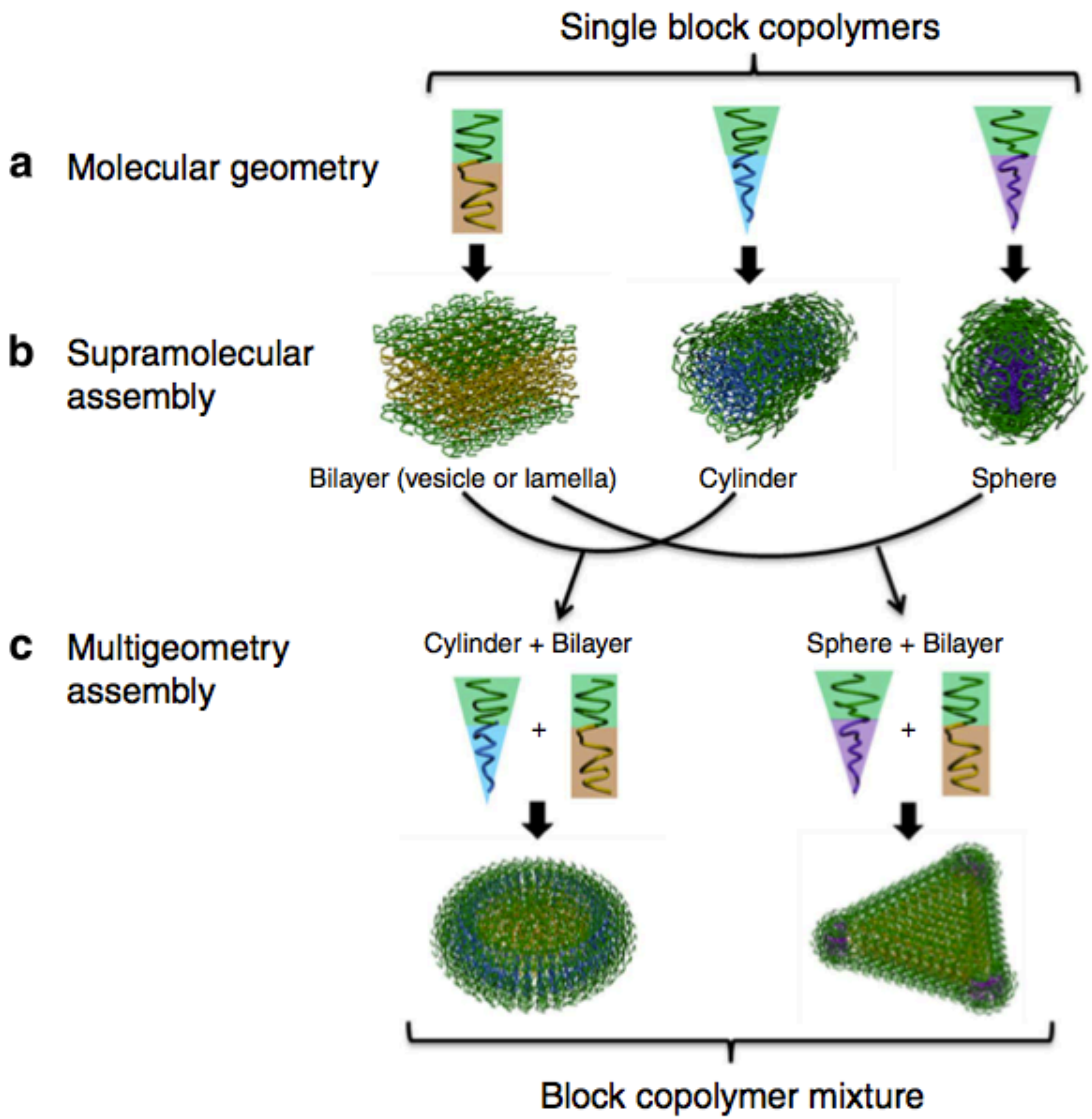


Block copolymers



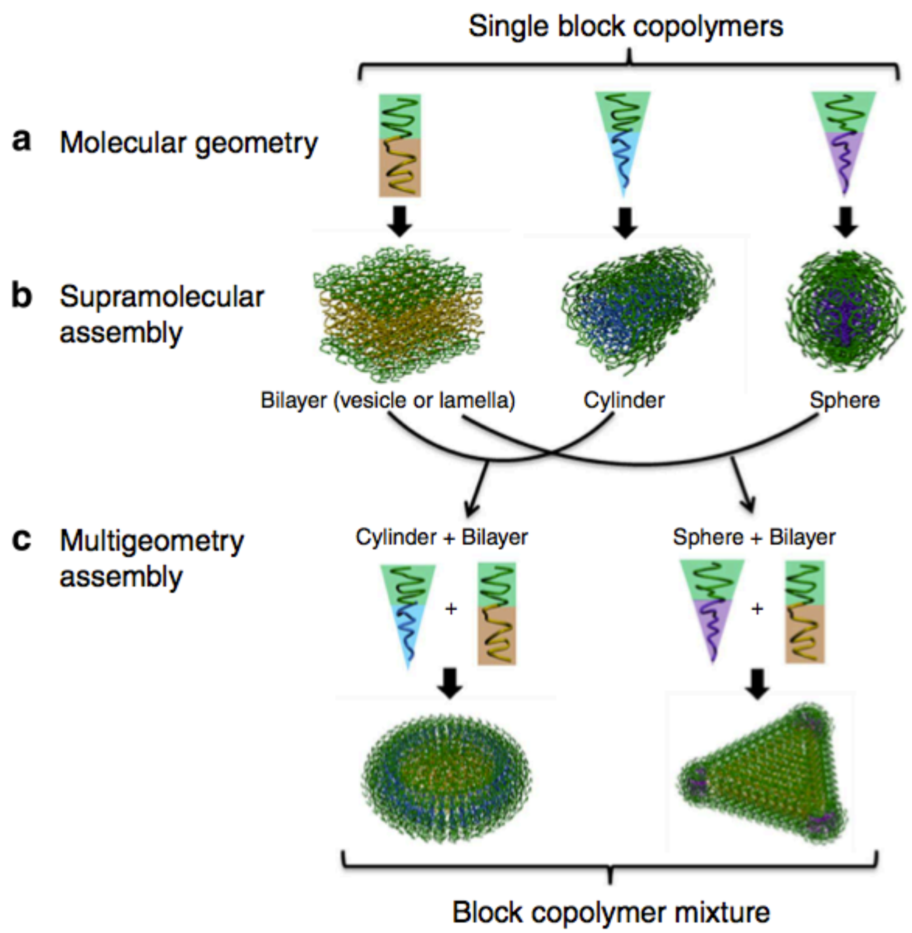
In solvent or in melt state

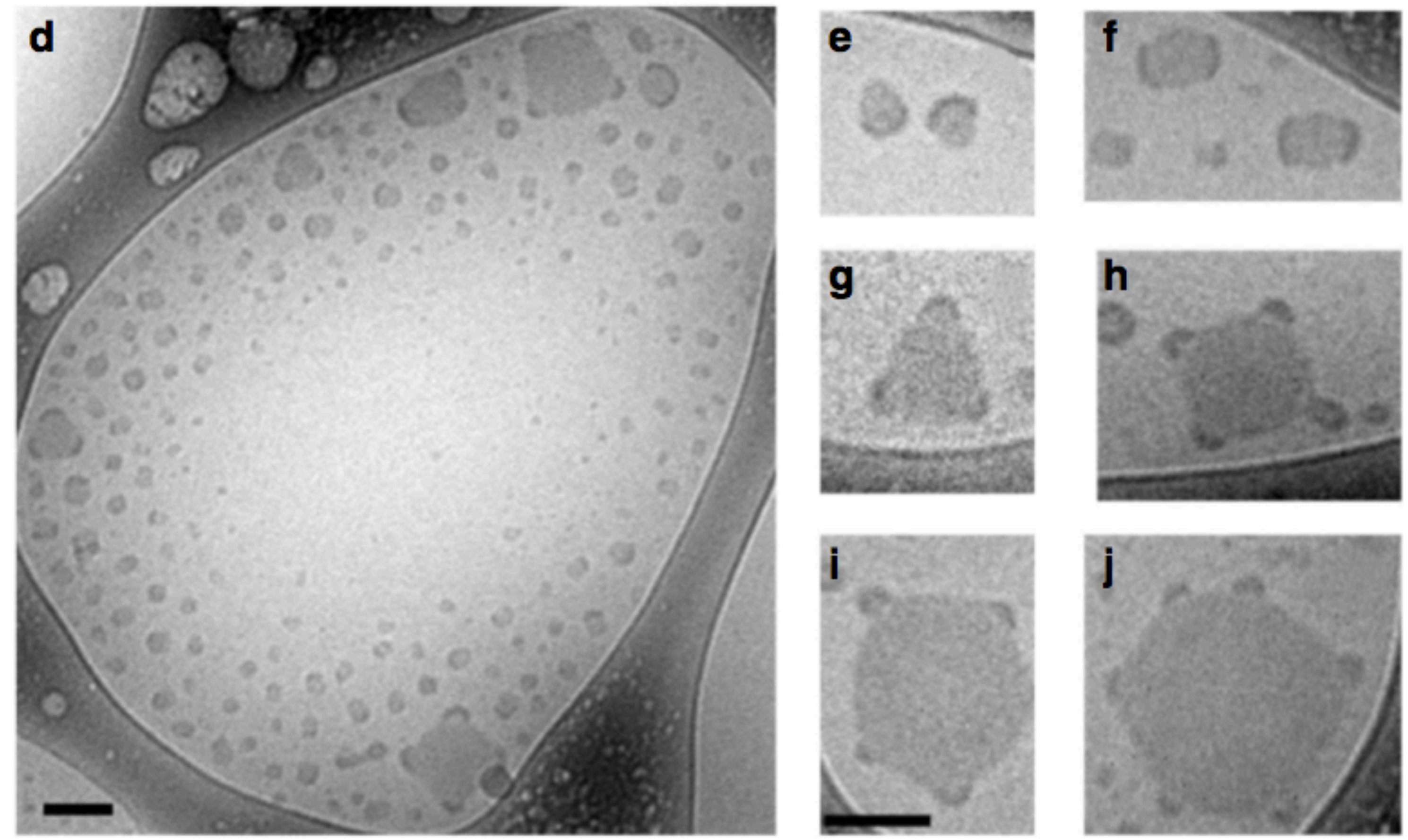
Dilute solution structures



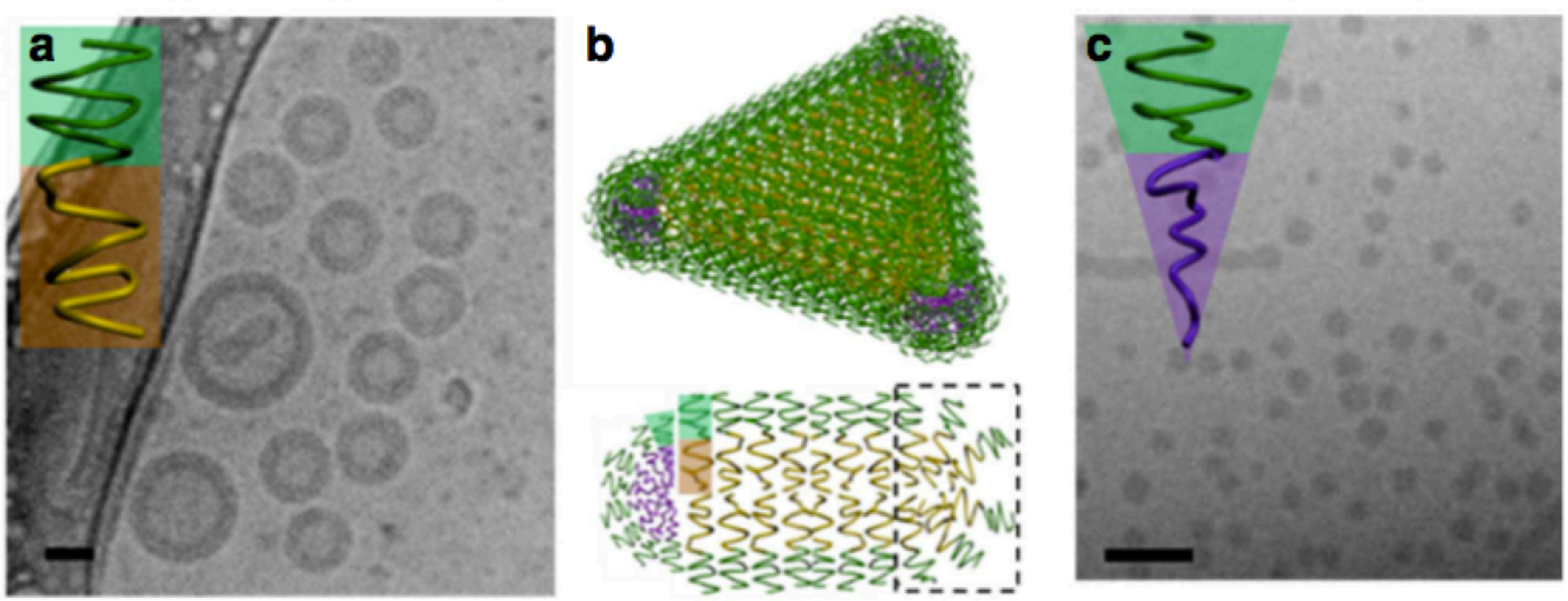
Zhu et al, Nature Comm., 4:2297, 2013

Dilute solution structures





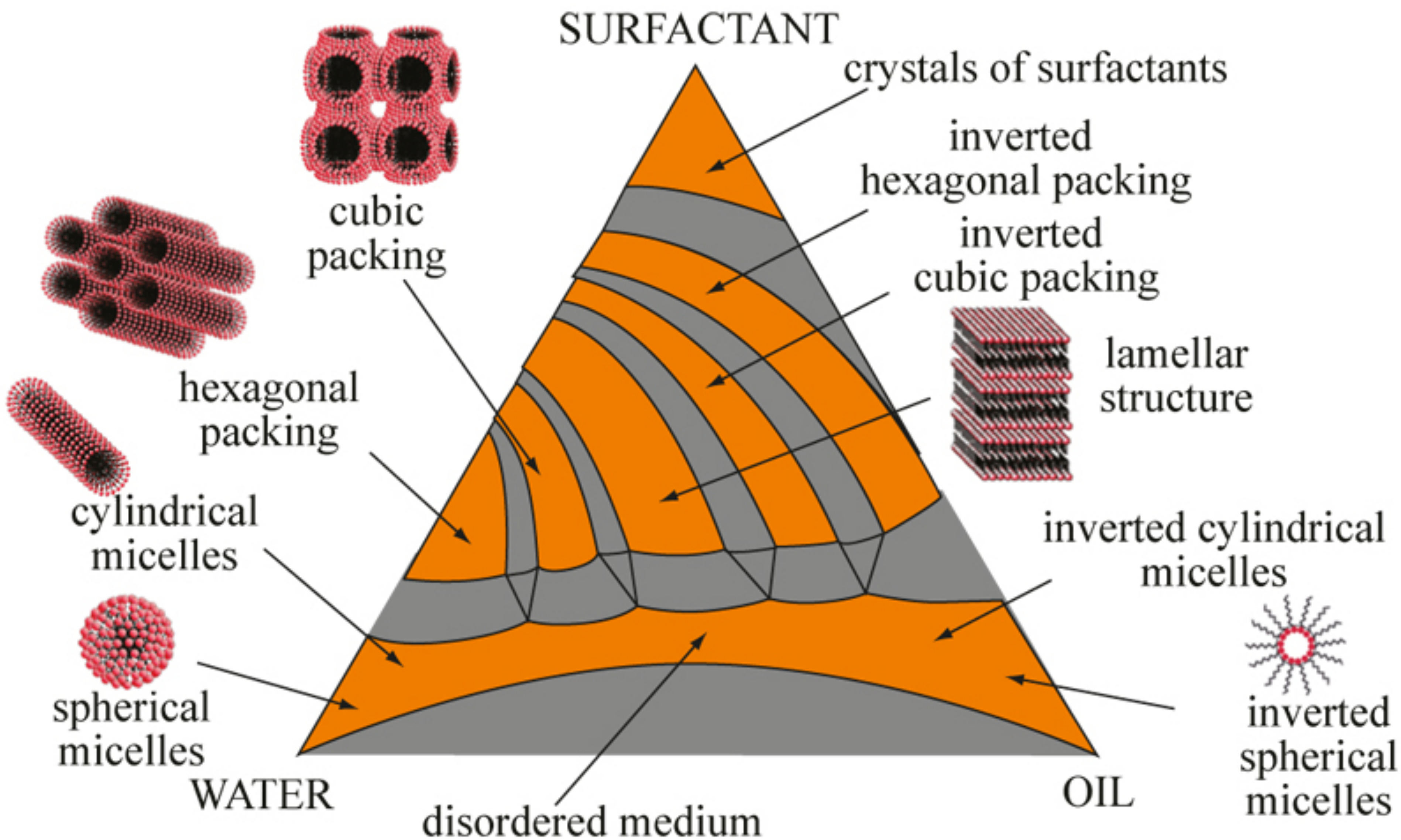
PAA$_{150}$-*b*-PMA$_{60}$-*b*-PS$_{240}$ PAA$_{75}$-*b*-PB$_{104}$

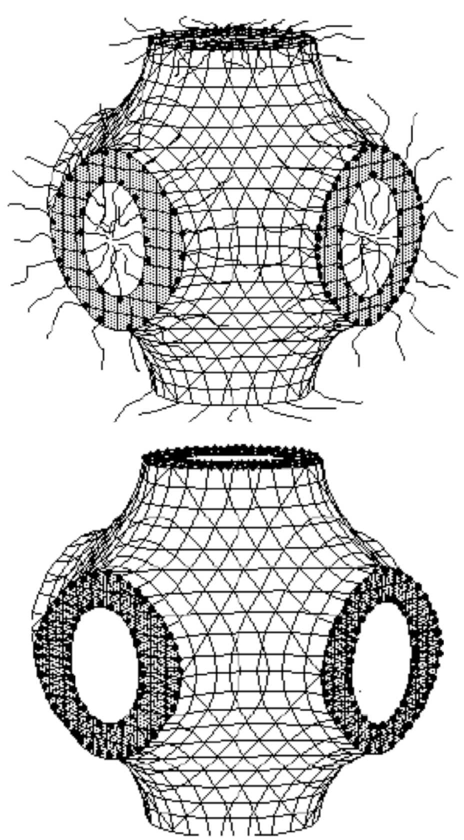


Scale bar, 100 nm.

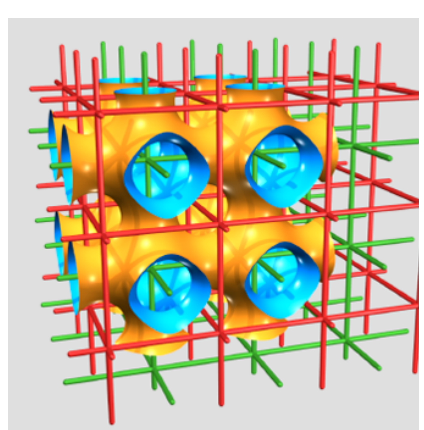
Zhu et al, Nature Comm., 4:2297, 2013

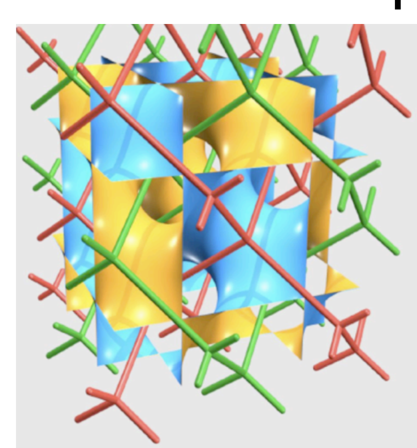
A surfactant phase diagram (in theory...)

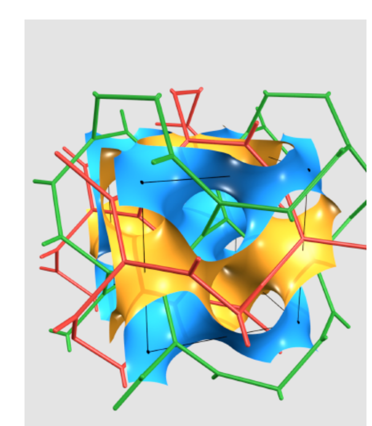




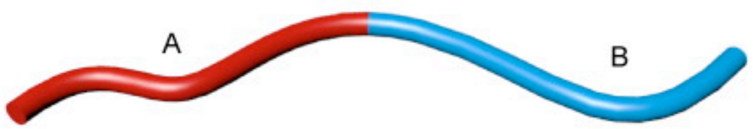
Bicontinuous cubic phases

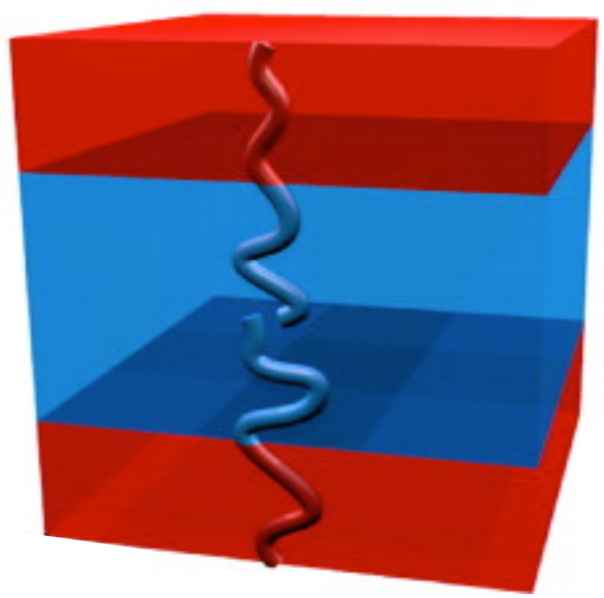


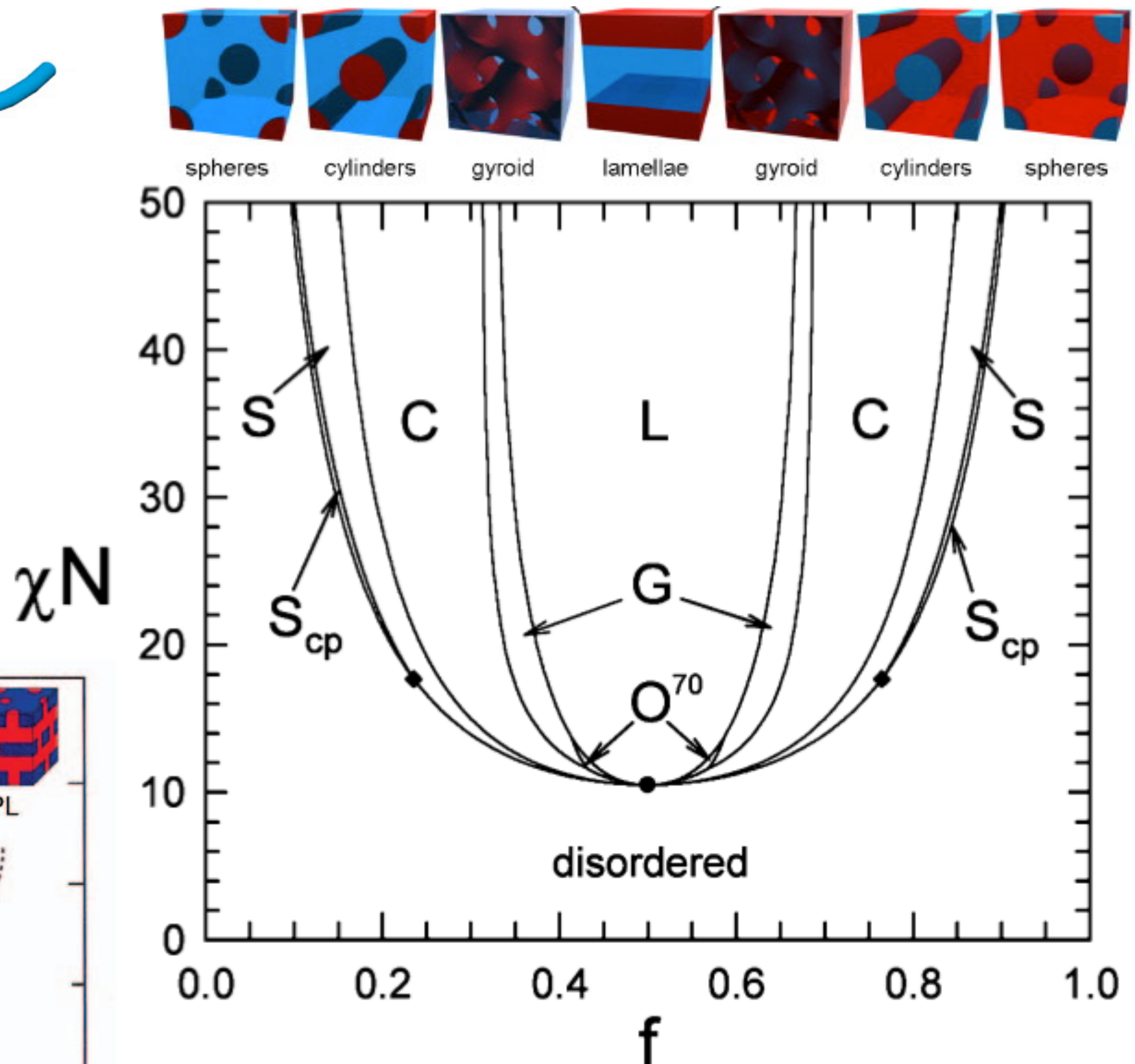


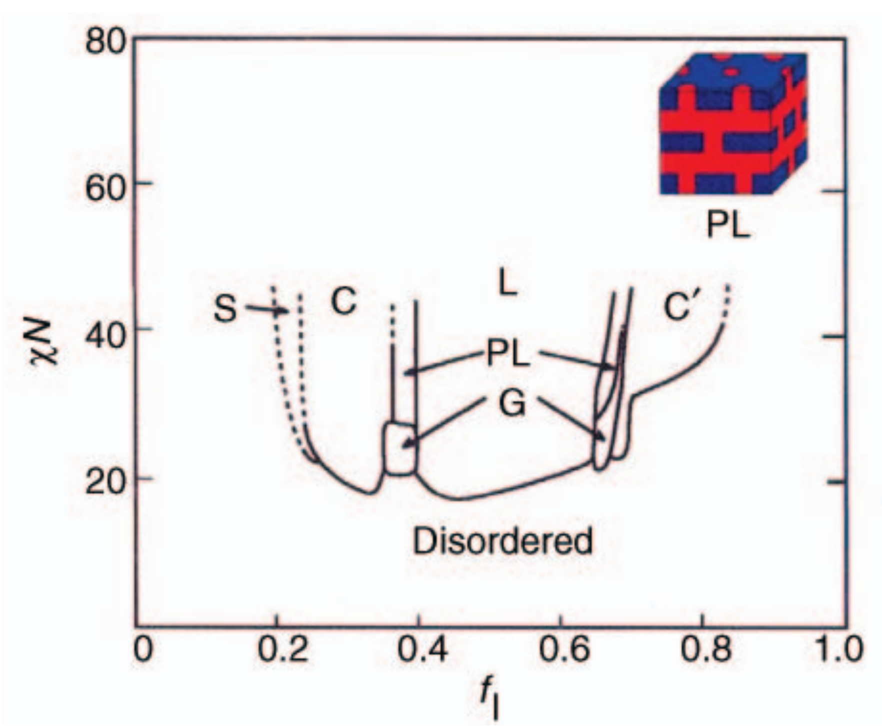


AB diblock copolymers



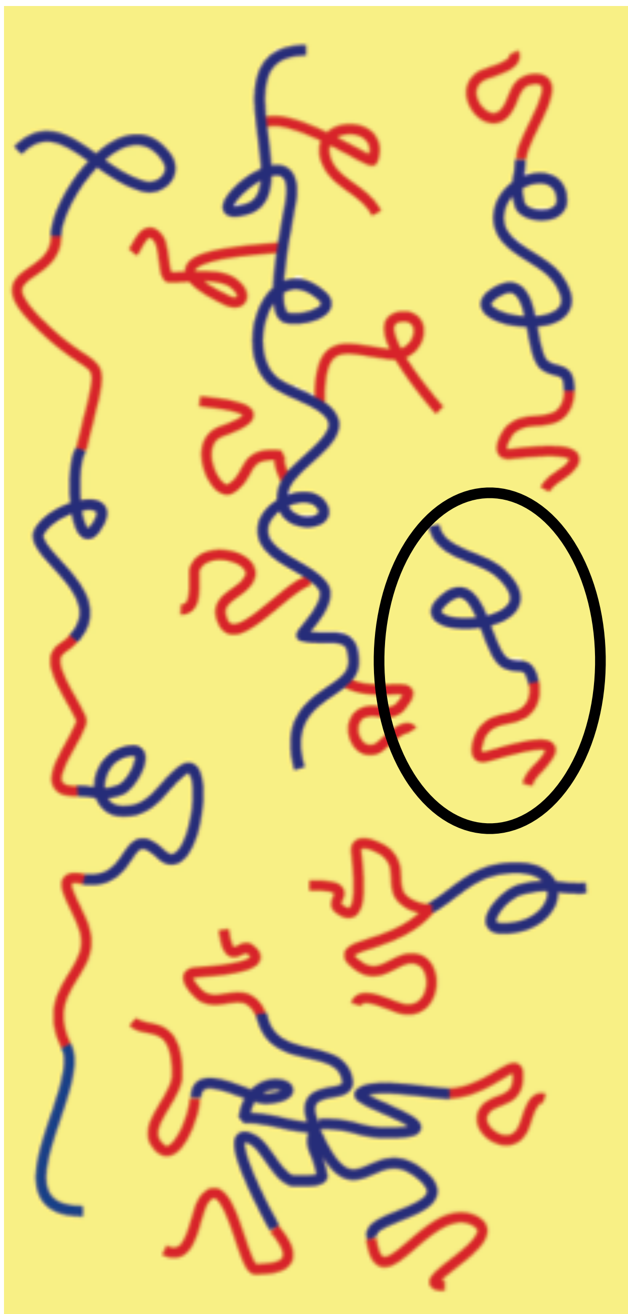


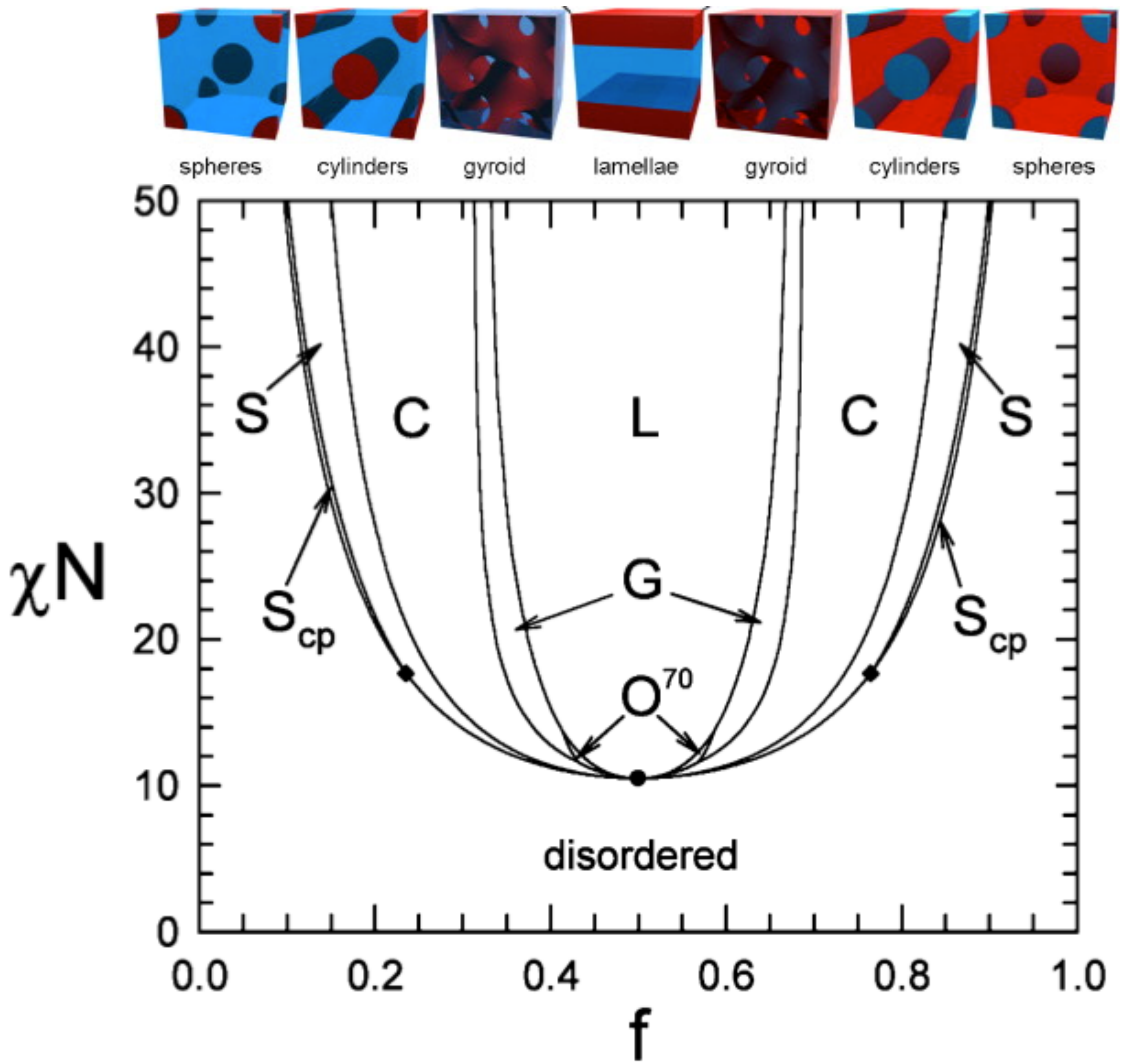




Matsen, *Macromolecules* 2012, 45, 2161–2165

AB copolymers: effect of molecular architecture





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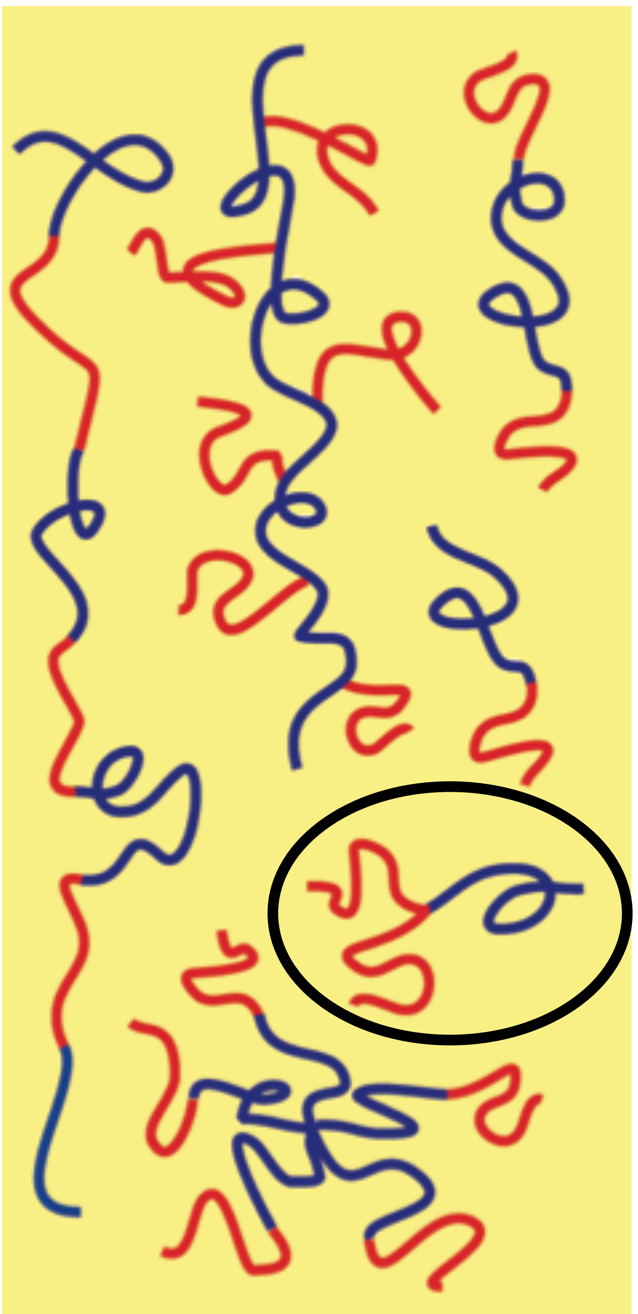
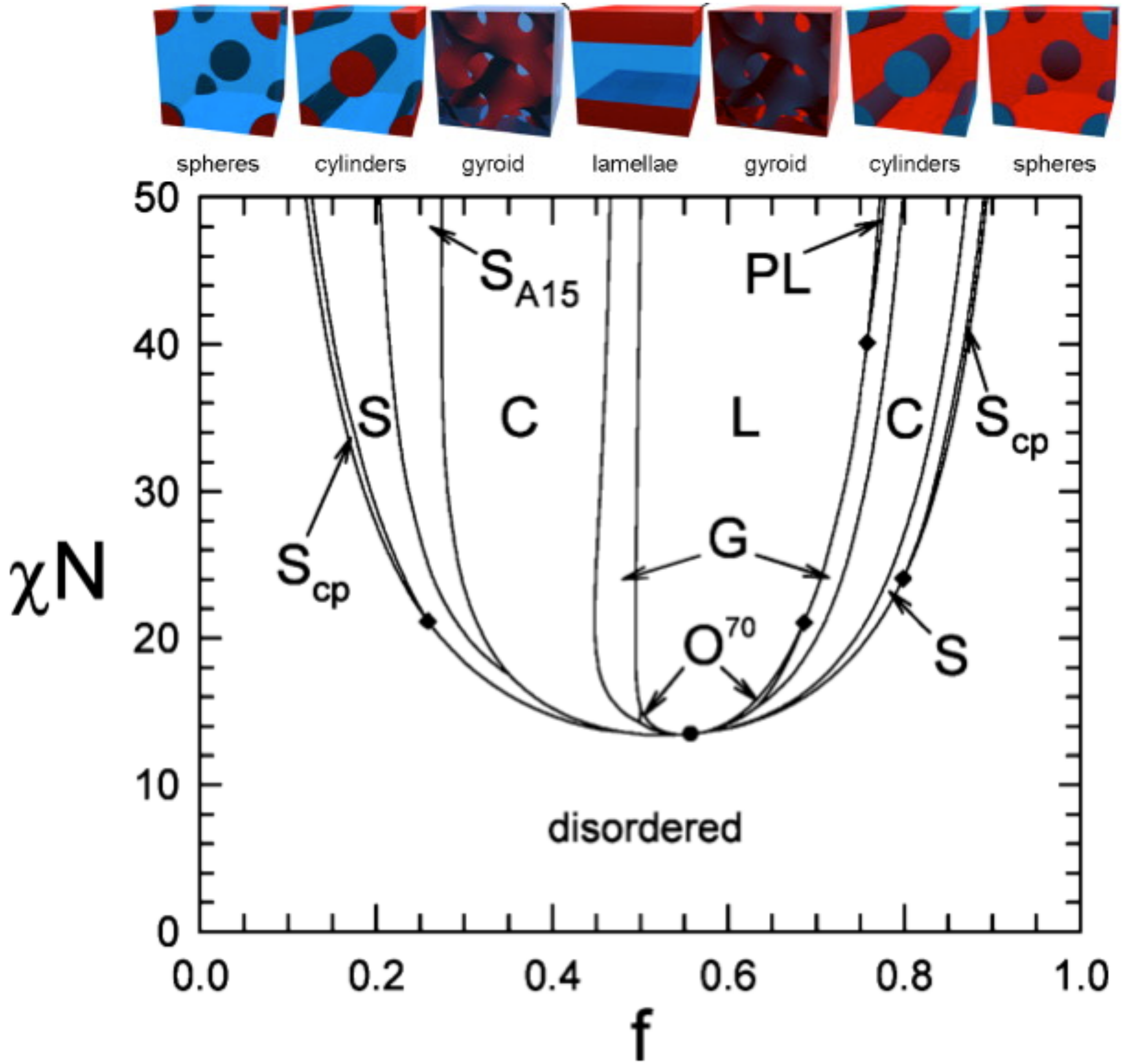
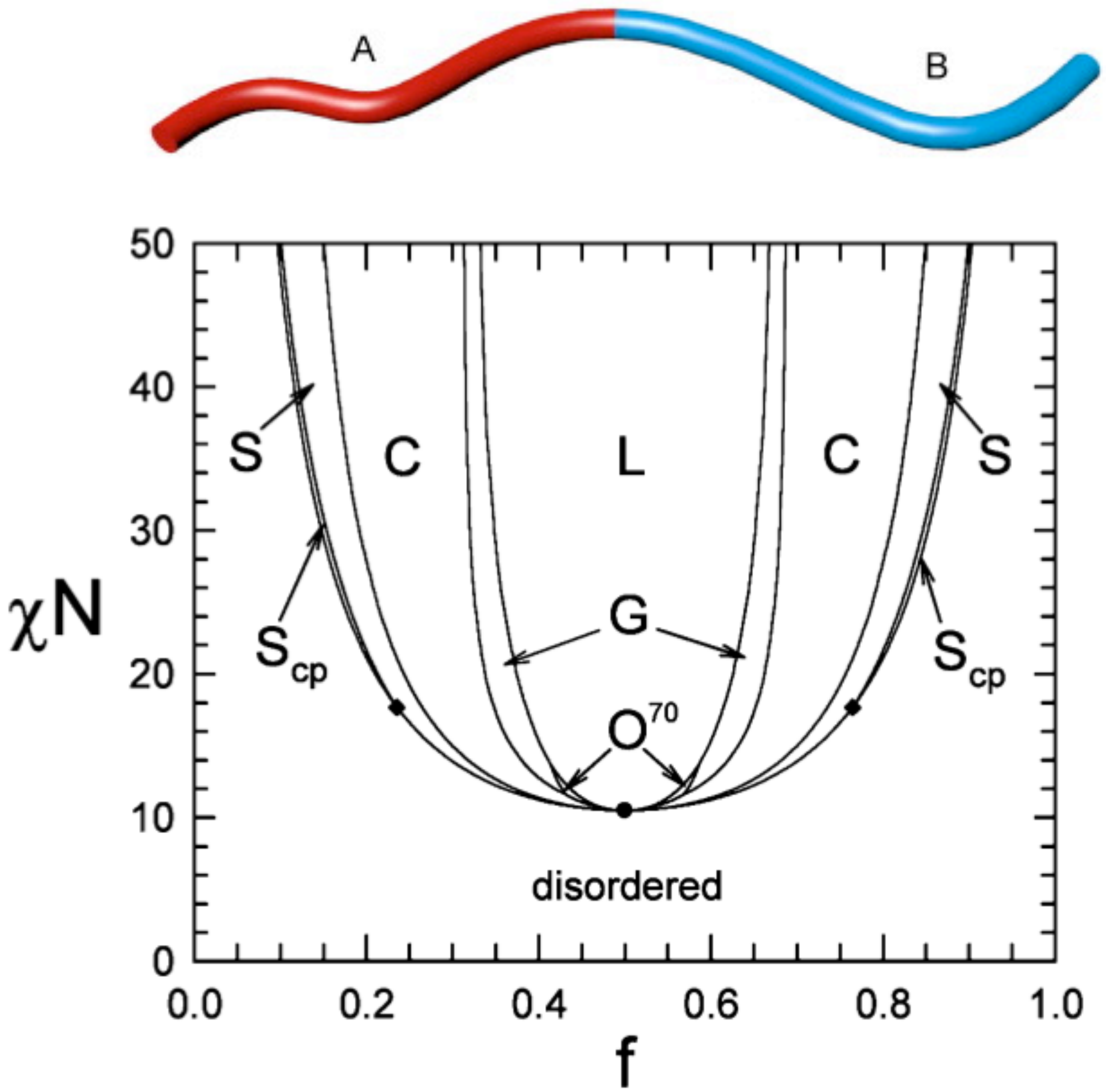




Matsen, *Macromolecules* 2012, 45, 2161−2165

Linear block copolymers: AB vs. ABC

AB diblock copolymer



Macromolecules 2012, 45, 2161−2165

ABC triblock copolymer

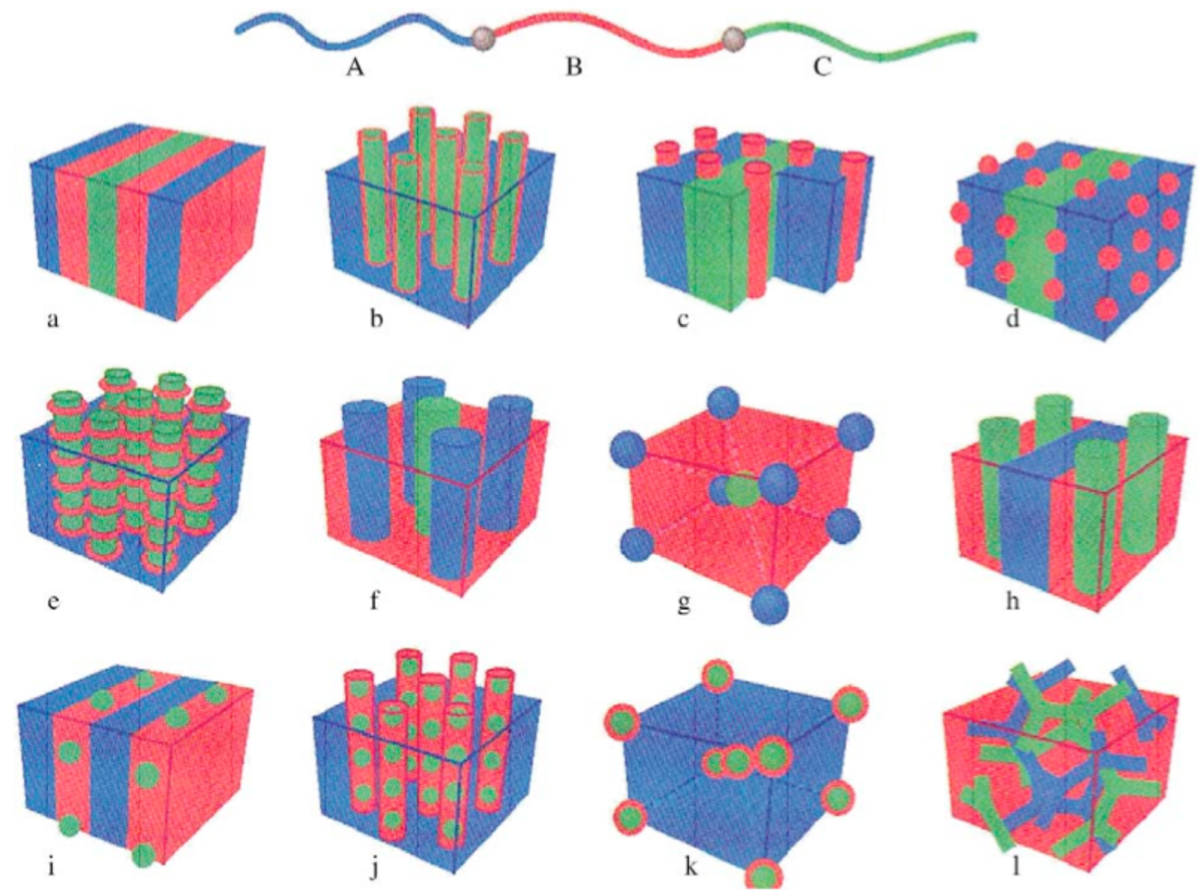
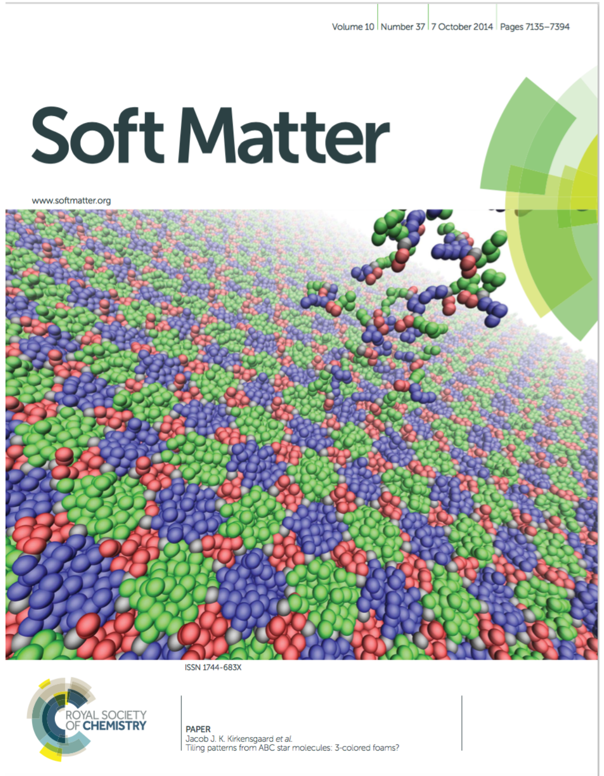


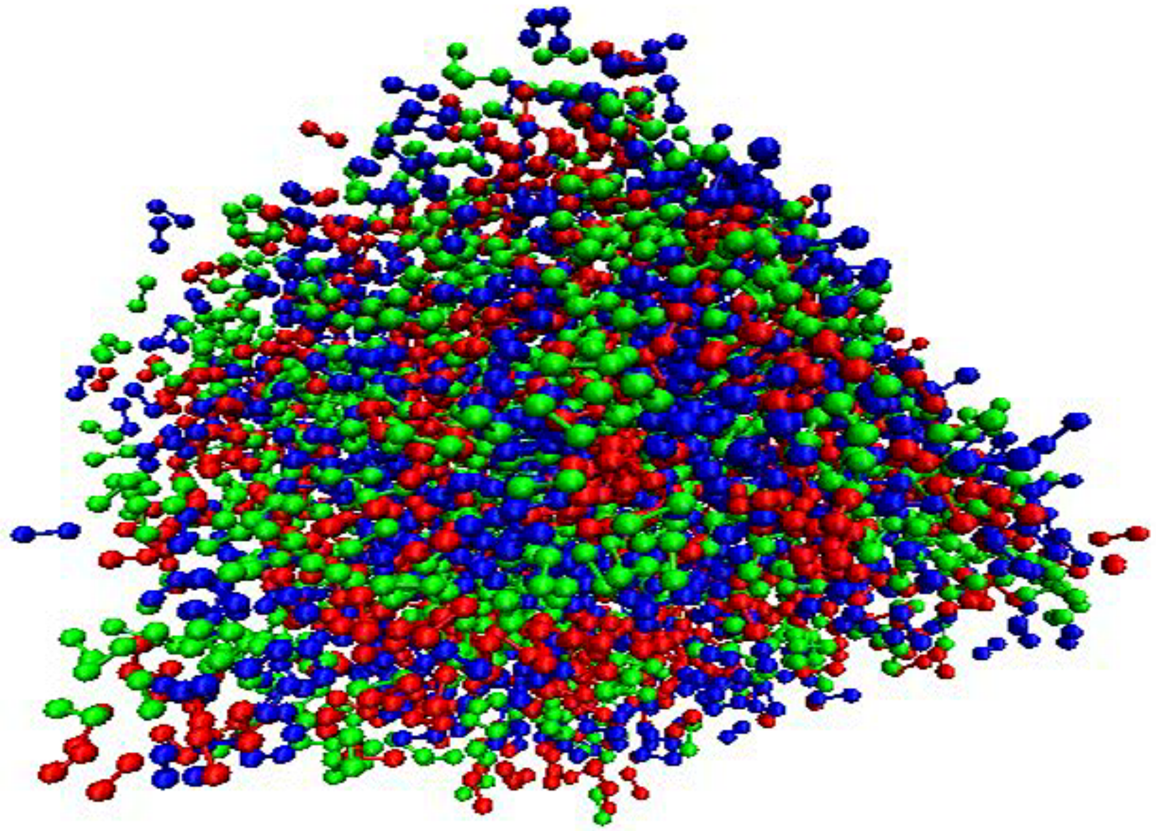
Figure from Hadjichristidis *et al.* 2005, Prog. Polym. Science 30

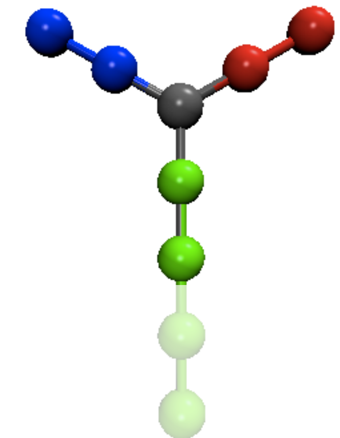
Same structural vocabulary

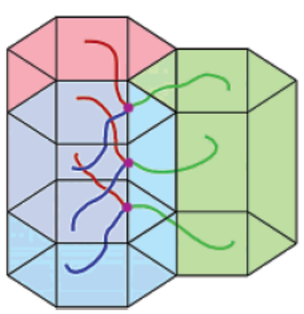
Interfaces = Surfaces



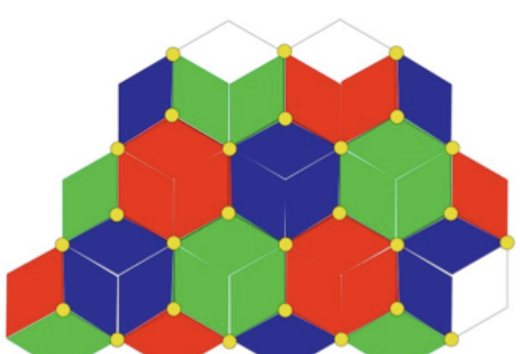
ABC star triblock terpolymers

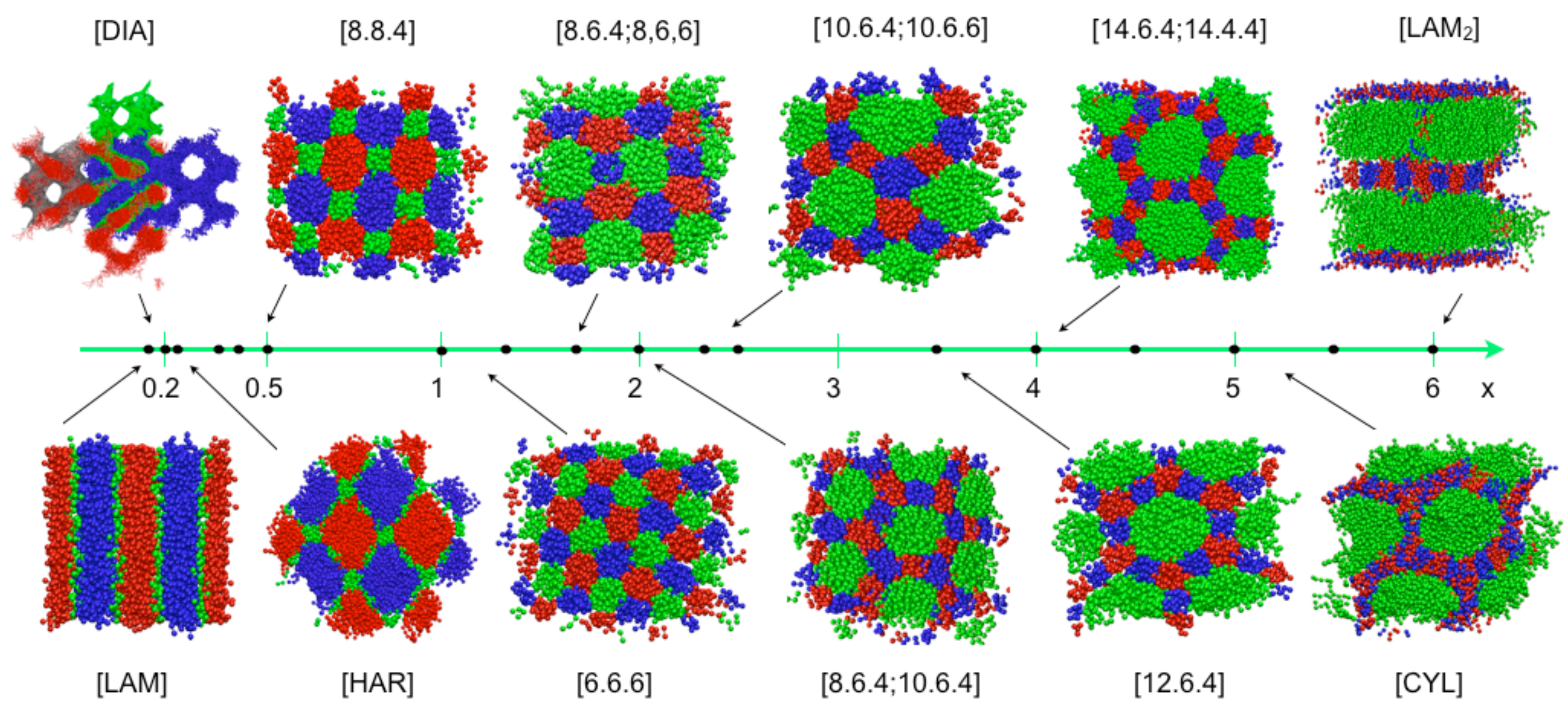






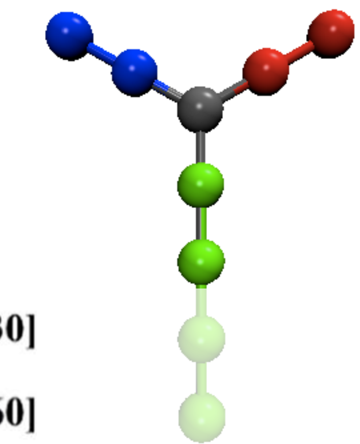
line torsion, curvature = 0.

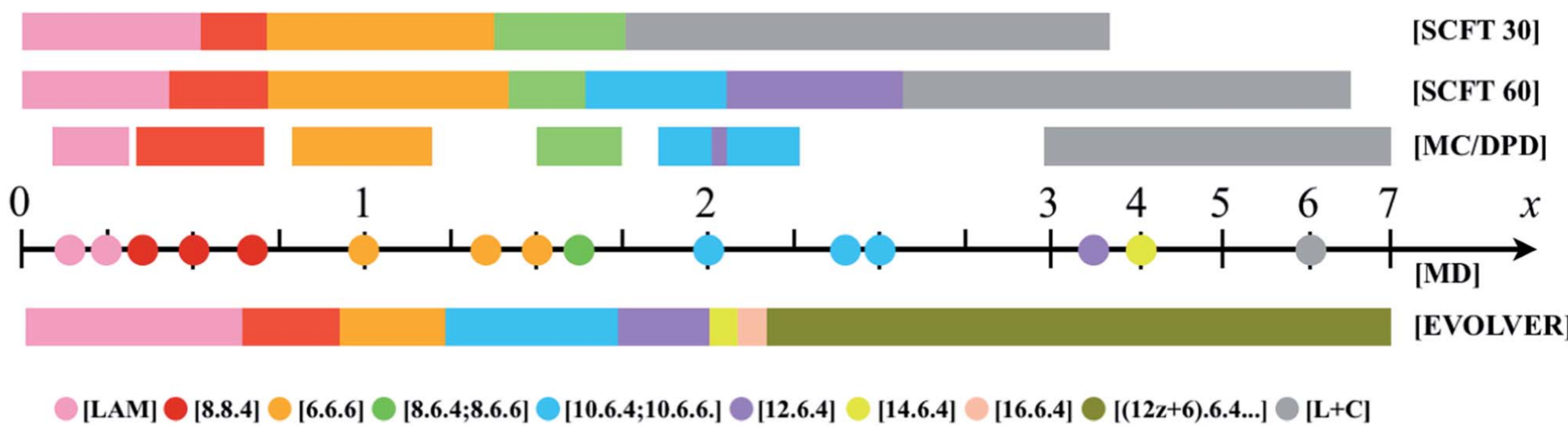


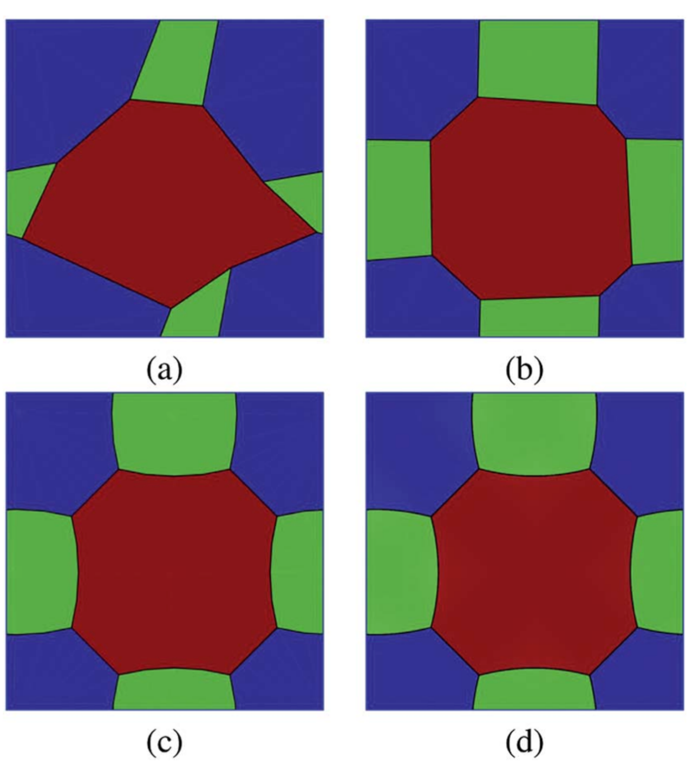


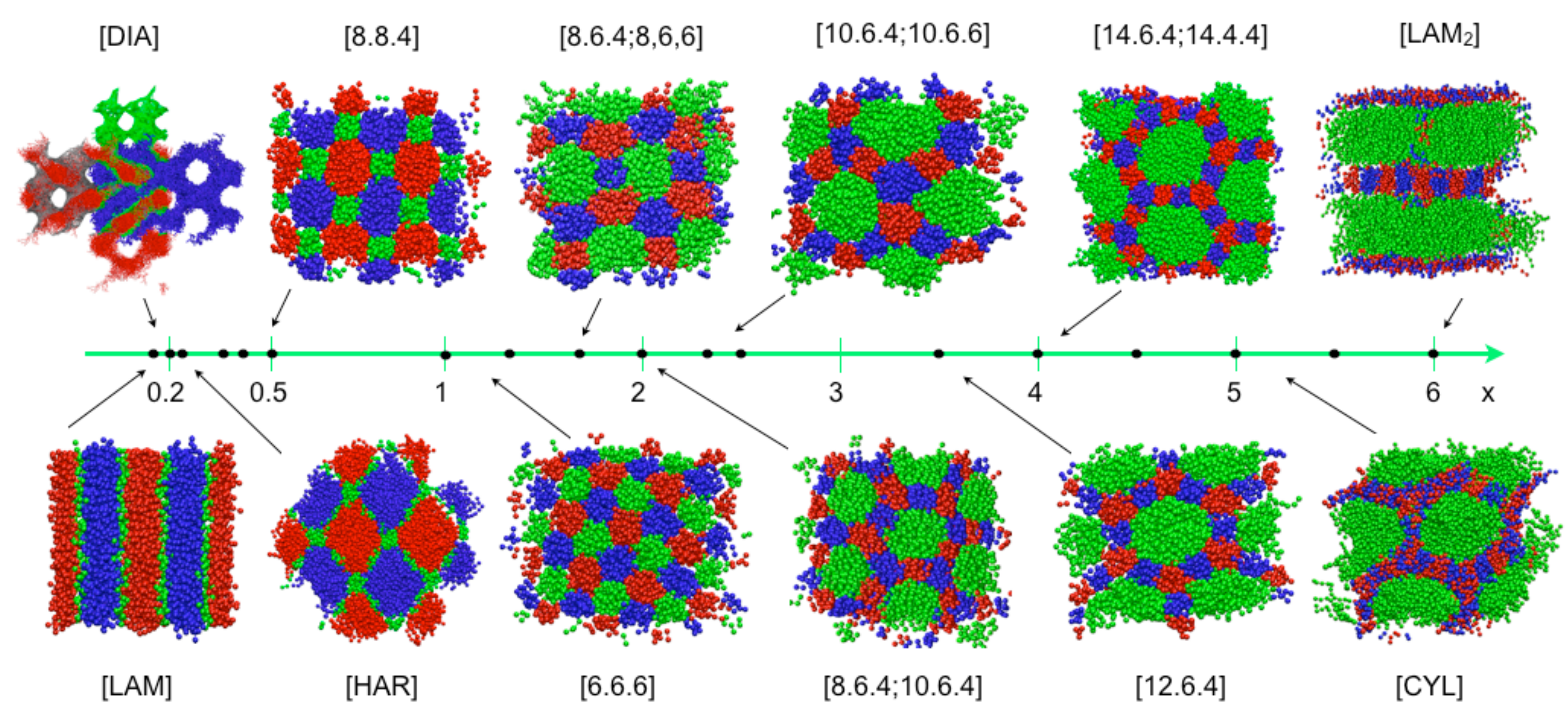
Kirkensgaard JJK, Pedersen MC and Hyde ST, Soft Matter, 2014, 10, 37, 7135

ABC star triblock terpolymers









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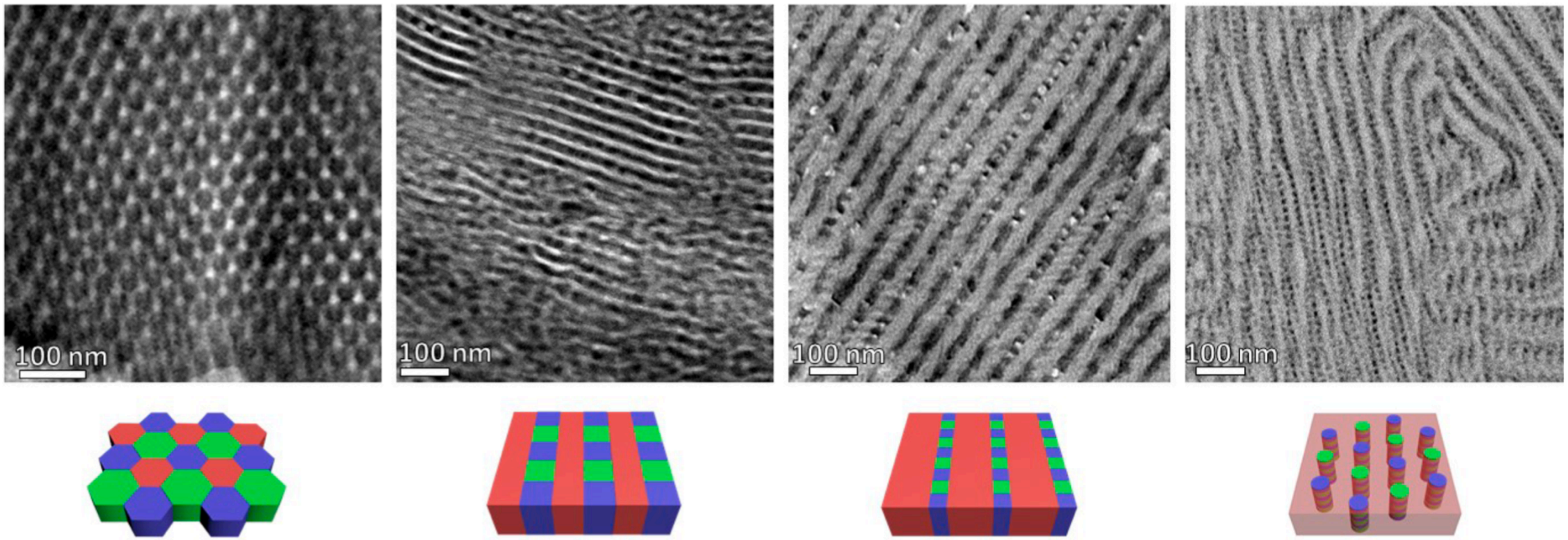
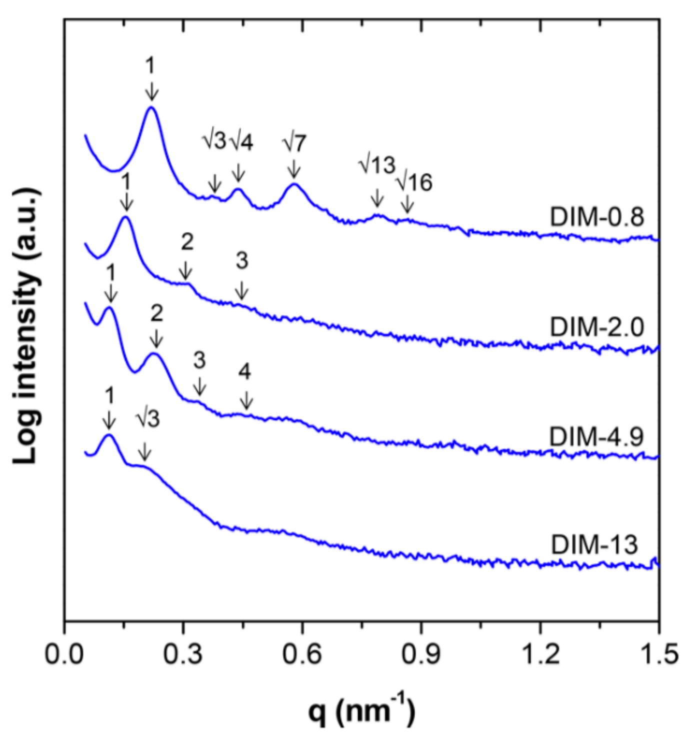
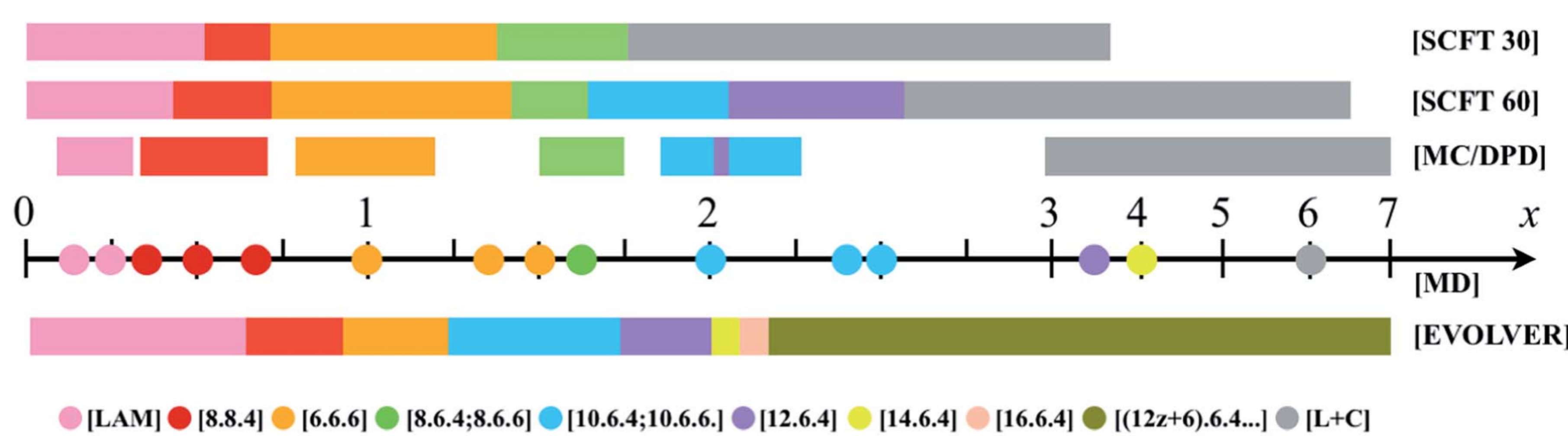
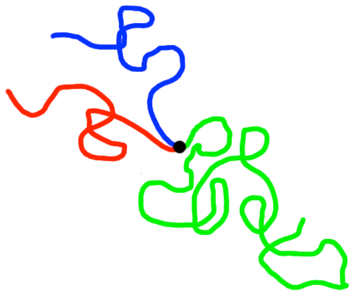


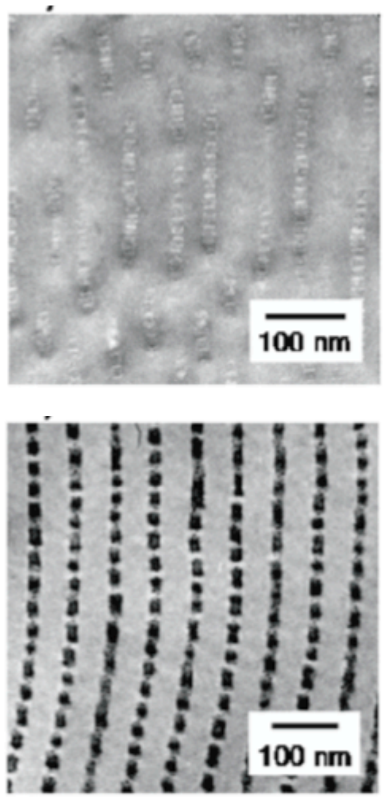


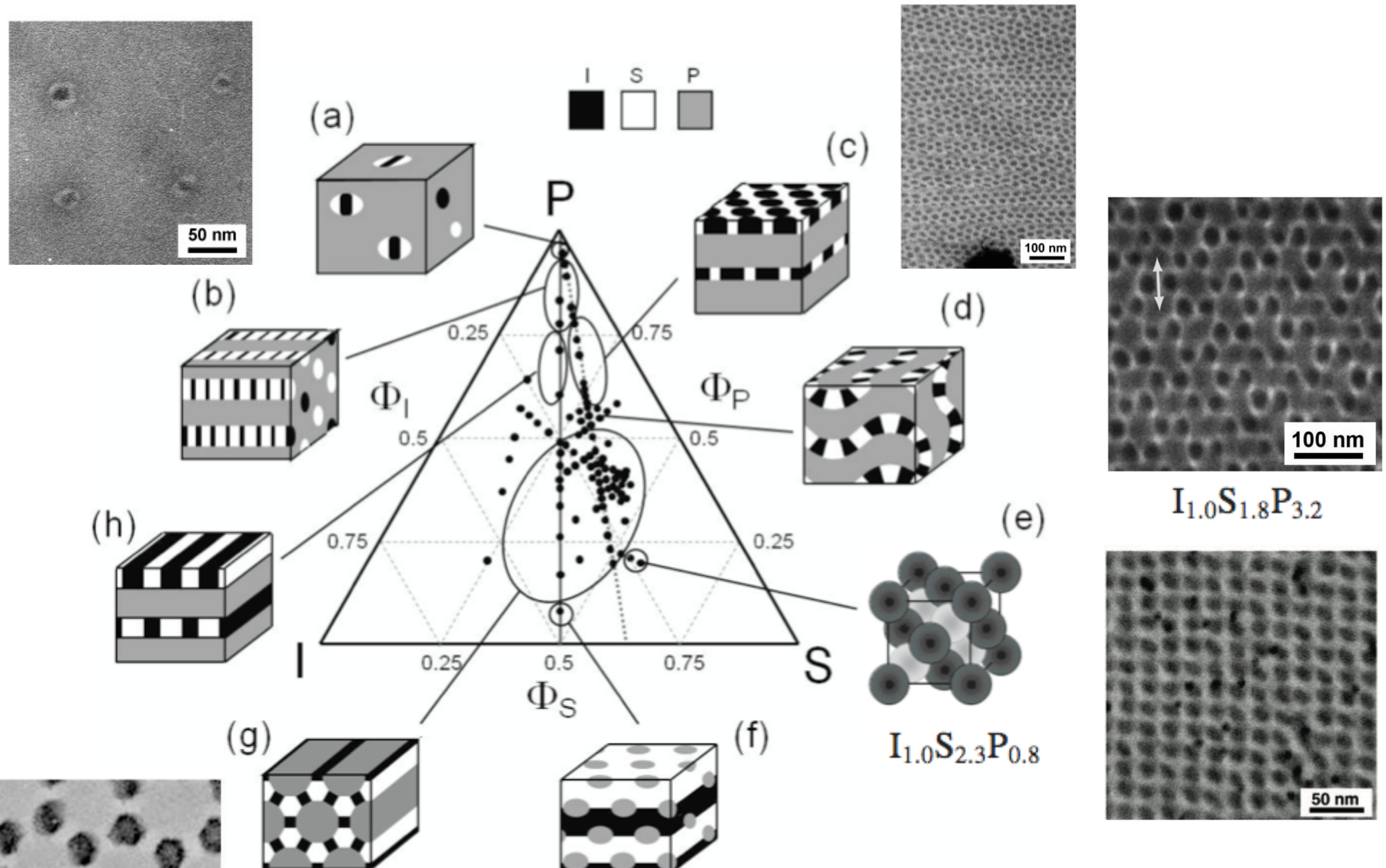


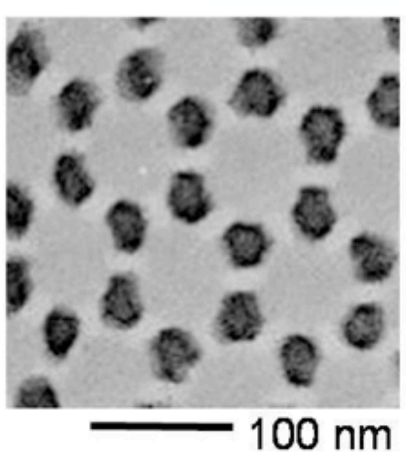
Chernyy, Kirkensgaard *et al.*
Macromolecules 2018, 51, 1041−1051

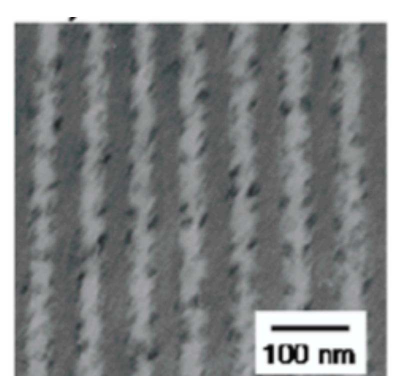


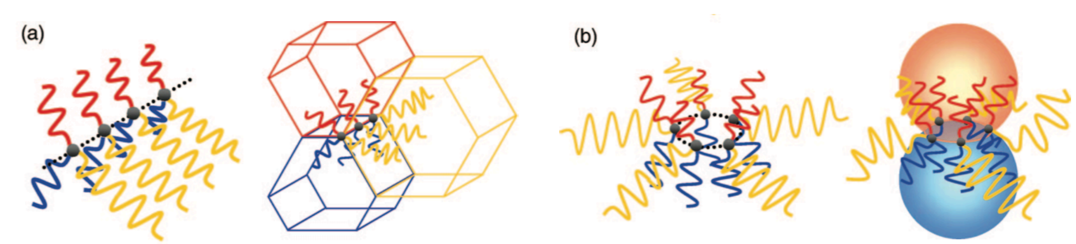
ABC stars - experimental ISP phase diagram





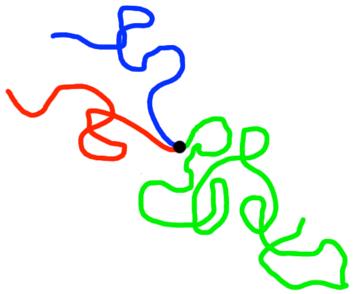




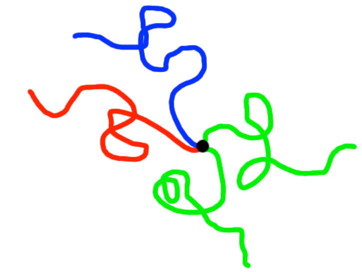


$I_1S_{1.8}P_{0.8}$ + S-homopolymer blend

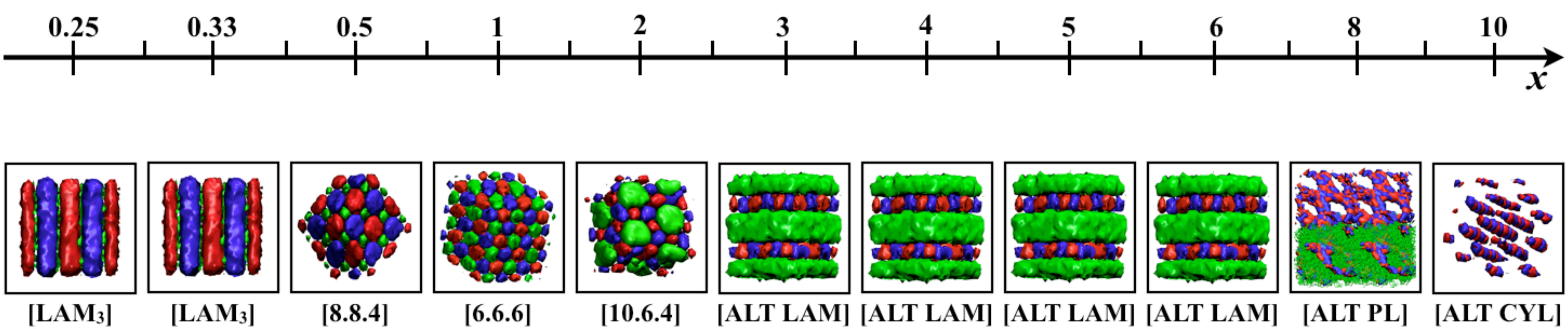
Matsushita, Hayashida, Dotera, Takano,
J. Phys. Cond. Mat., 2011, 23, 284111



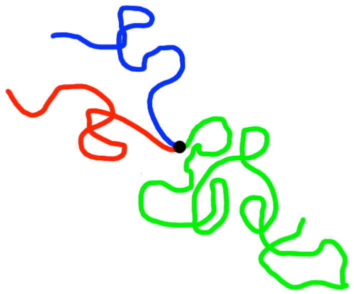
ABC_x vs ABC_n



Both $x = 2$ but molecular architecture differs



Kirkensgaard JJK, Phys Rev E, 85, 031802 (2012)



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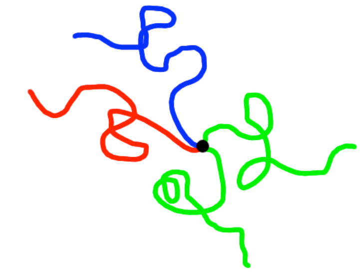

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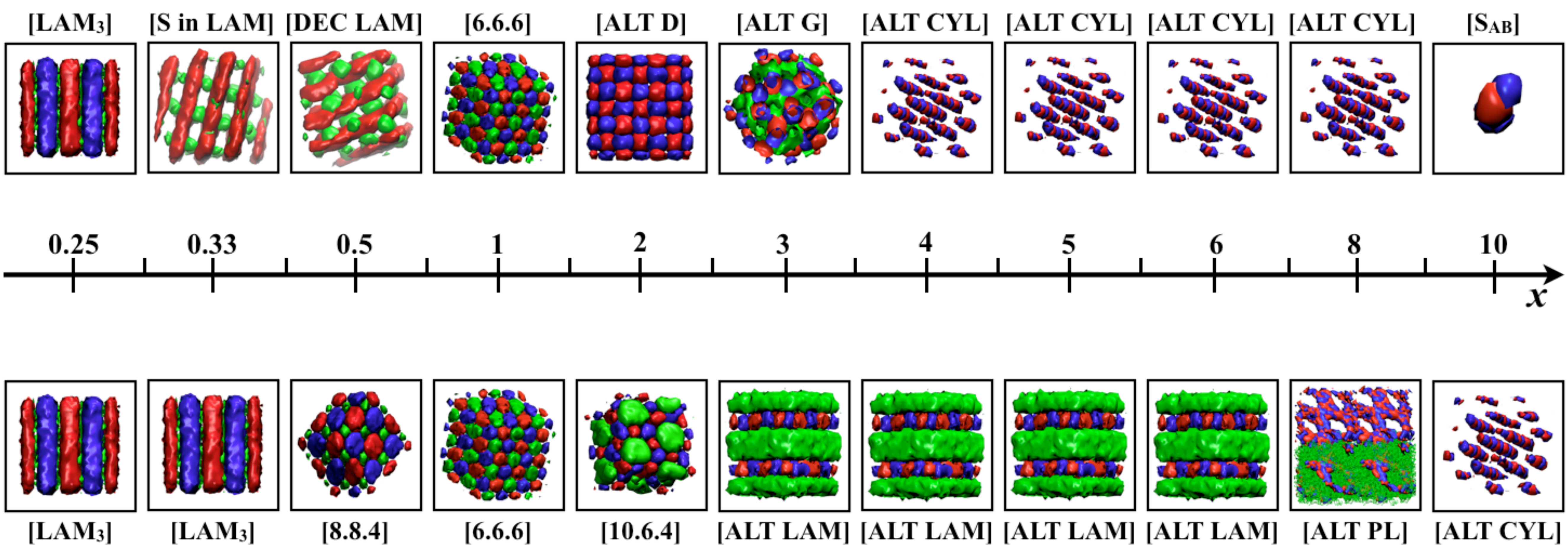

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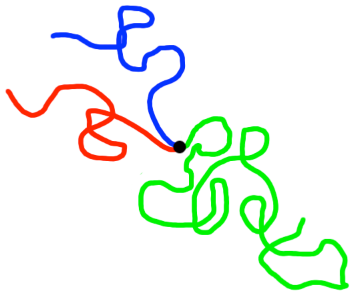
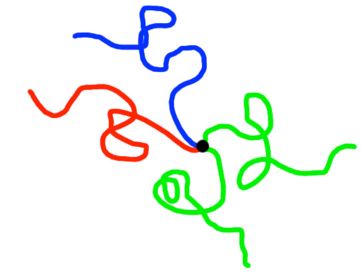
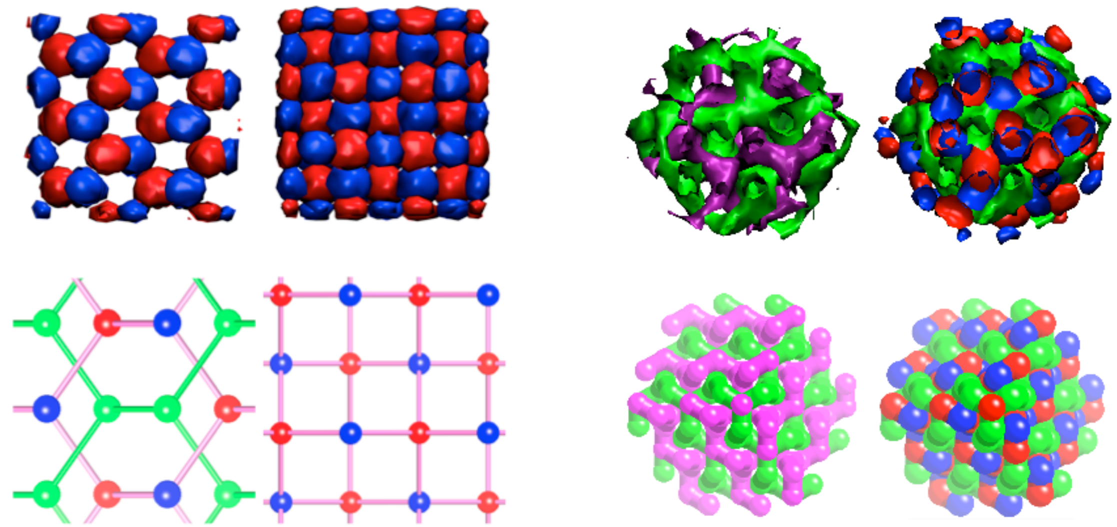
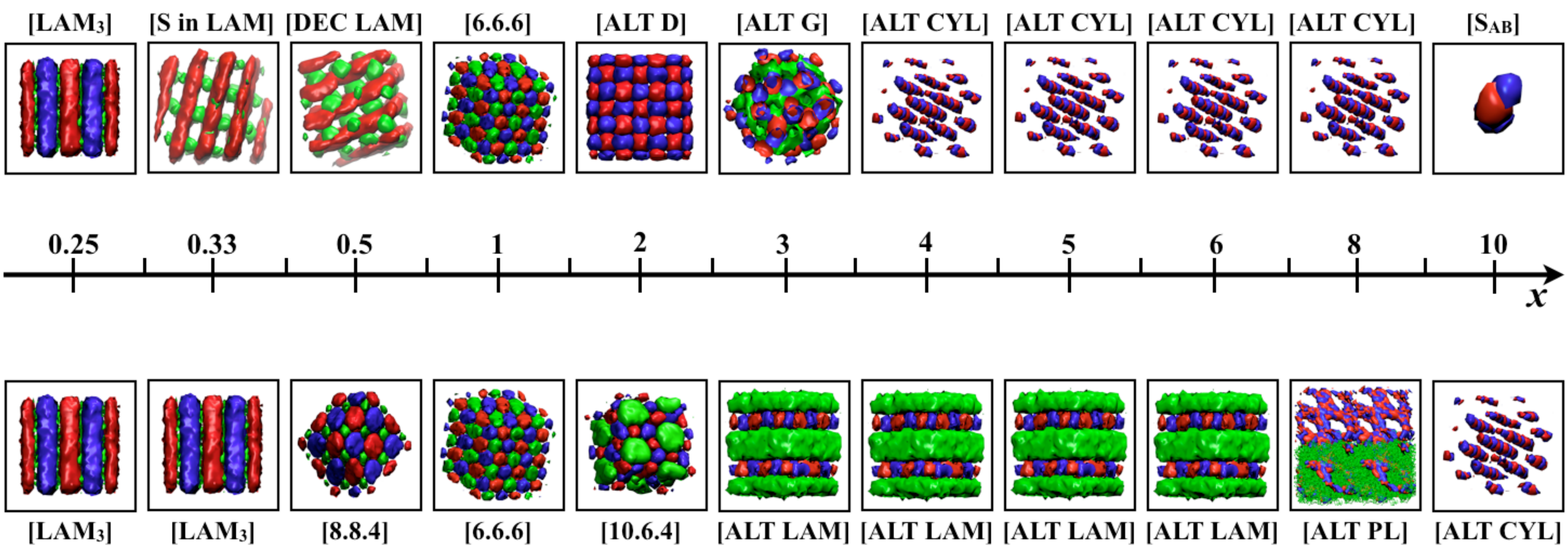


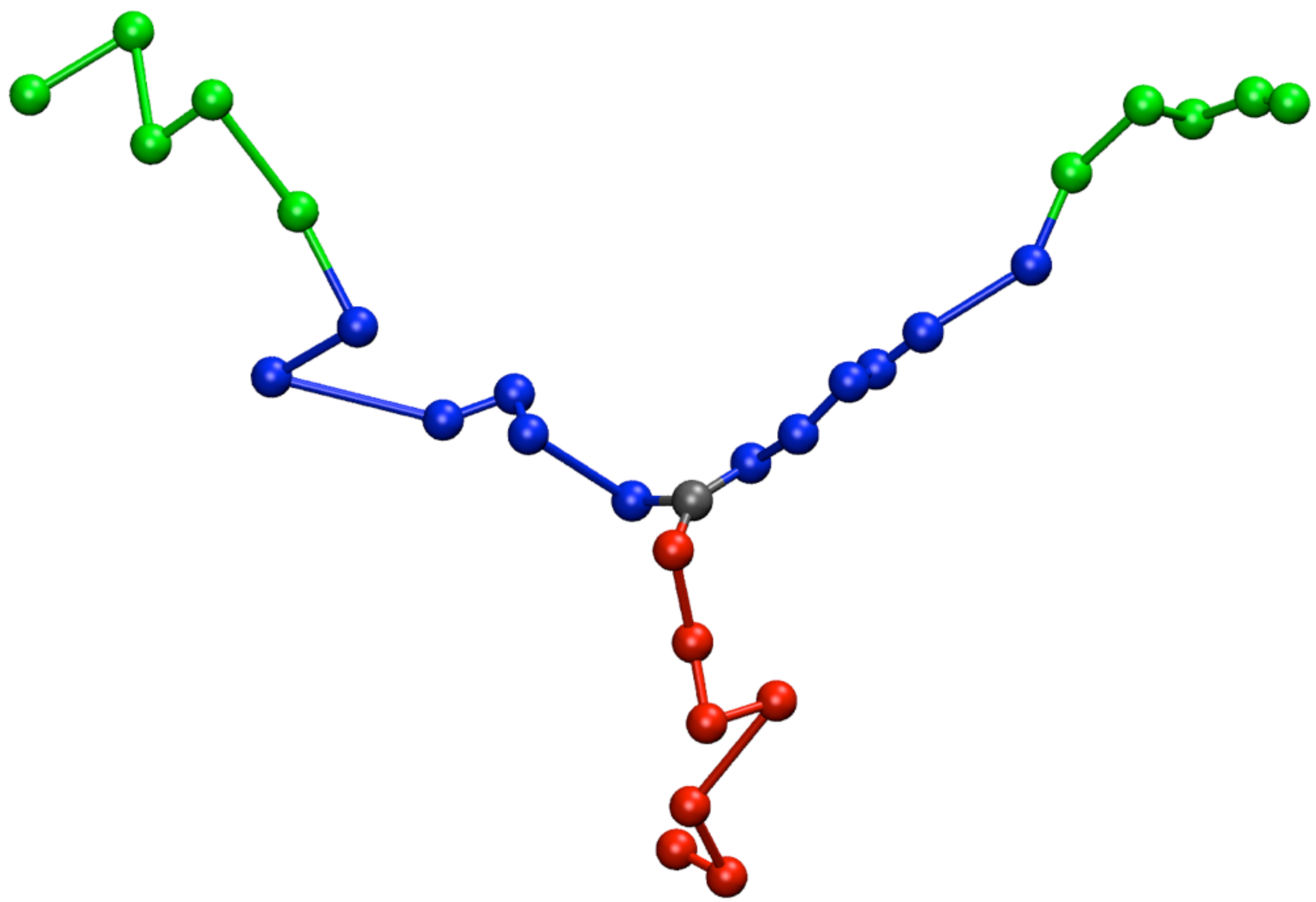




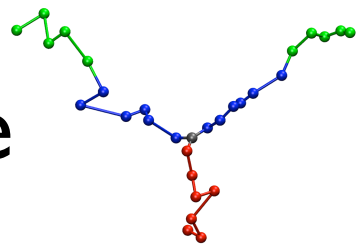


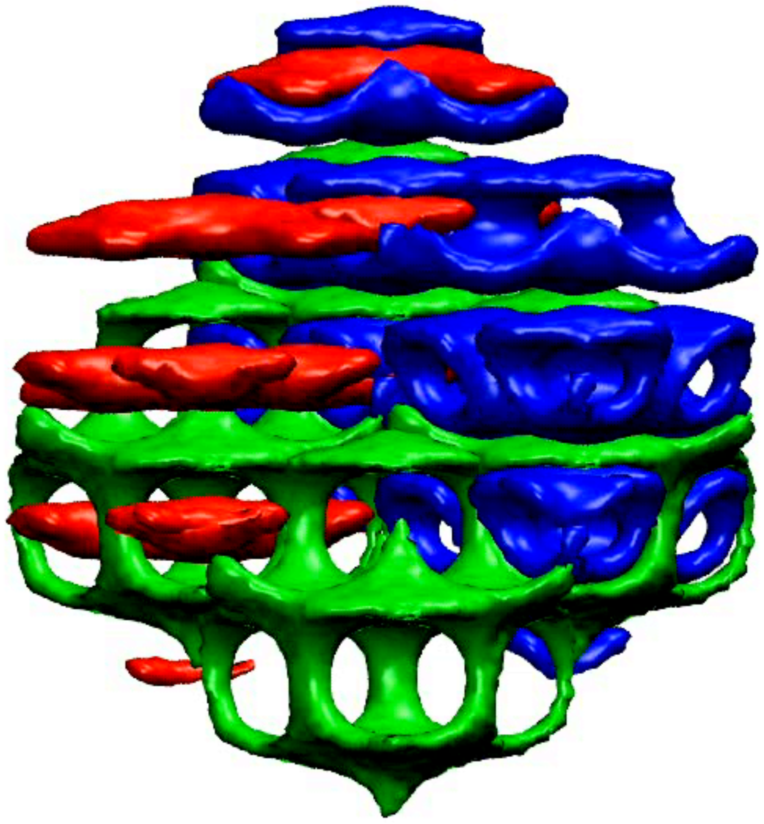
Kirkensgaard JJK, Phys Rev E, 85, 031802 (2012)

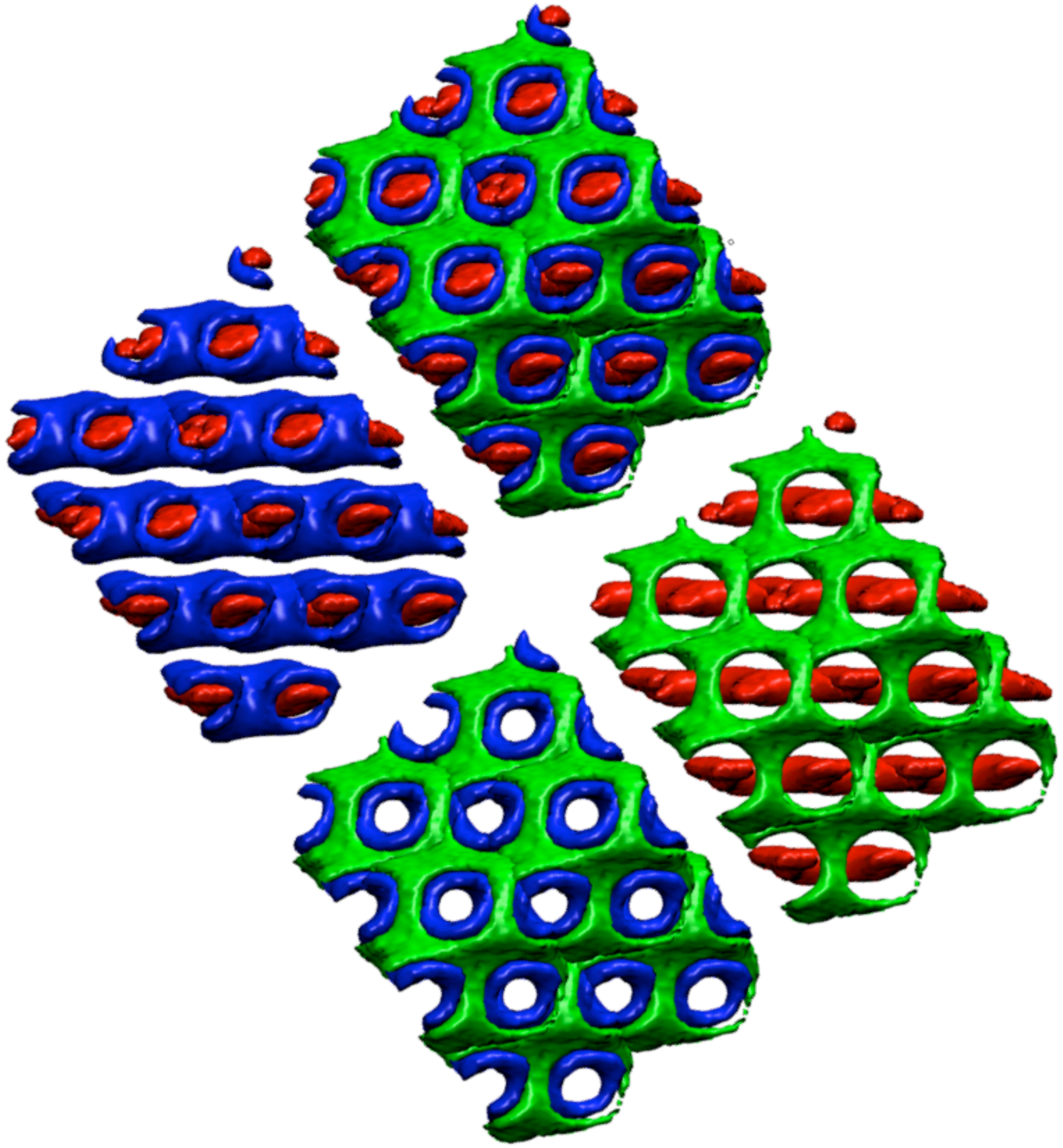
A(BC)$_2$ mikto-arm star copolymer



Self-assembly of A_7-$(B_6$-$C_5)_2$ reference structure



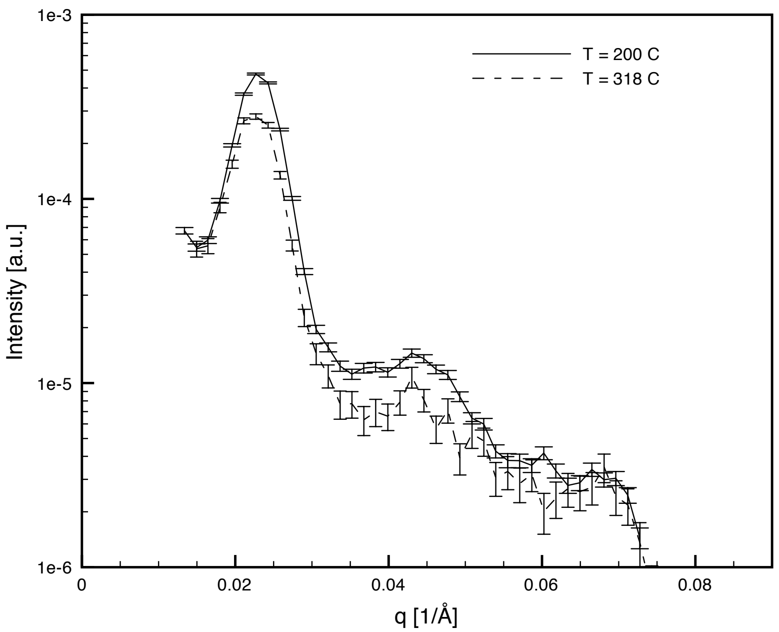




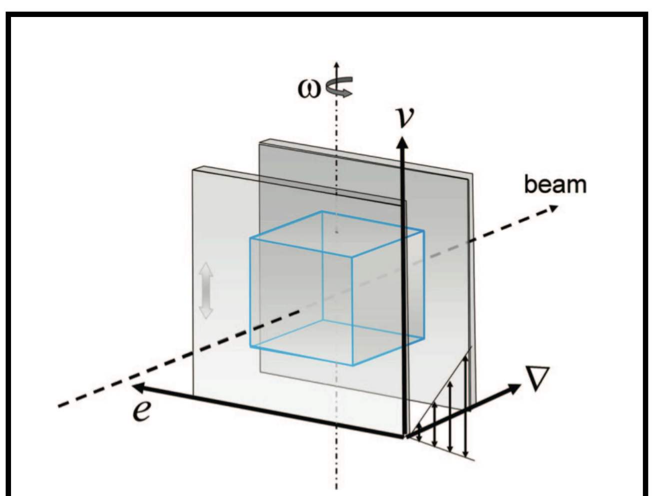
[PL_A] phase

Simulations: Kirkensgaard JJK, *Soft Matter*, 2010, 6, 6102-6108
Experimental: Kirkensgaard JJK, Fragouli P, Hadjichristidis N and Mortensen K *Macromolecules*, 2011, 44 (3), 575-582

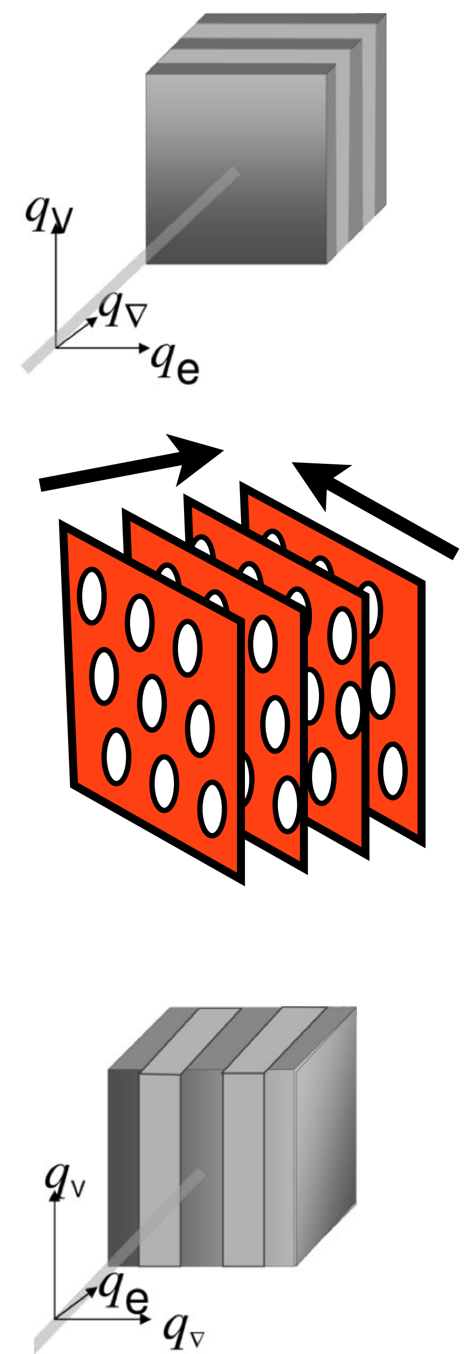
Rheo-SANS experiments support the PL structure

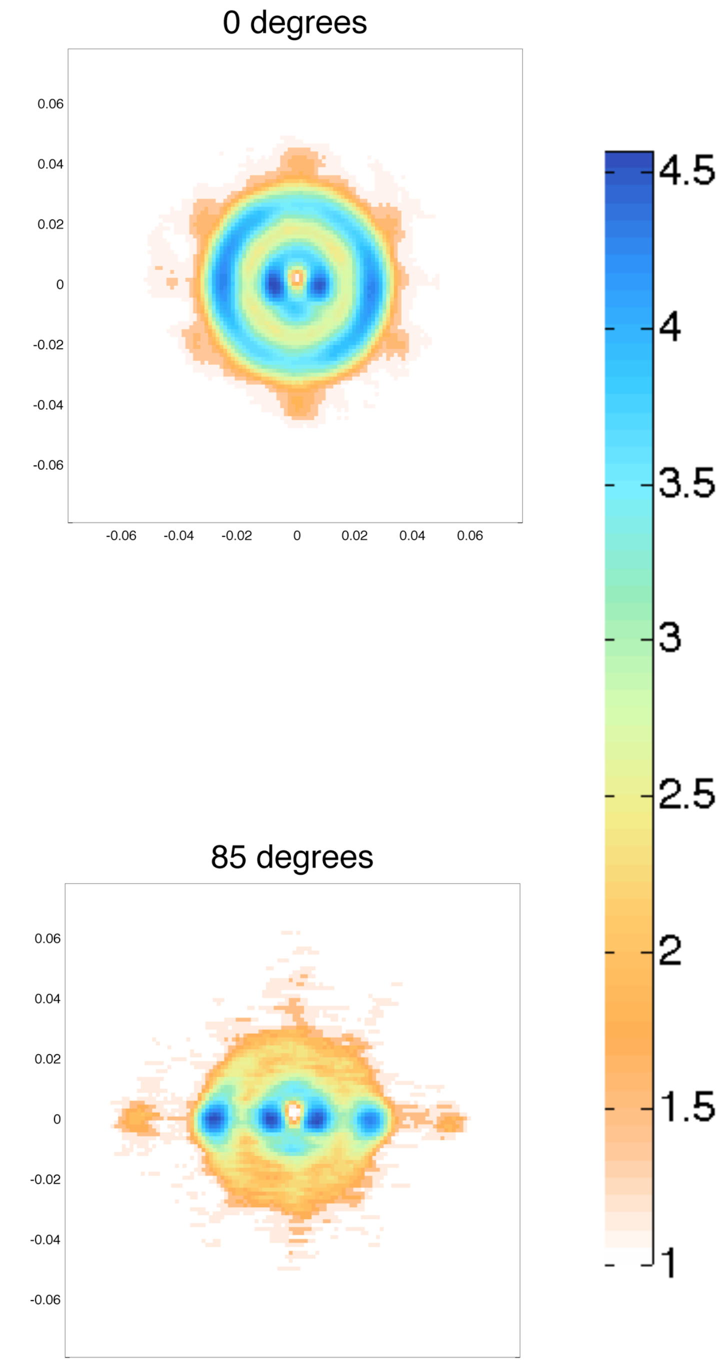


Non-aligned sample: q* ~ 0.023 => D ~ 275 Å



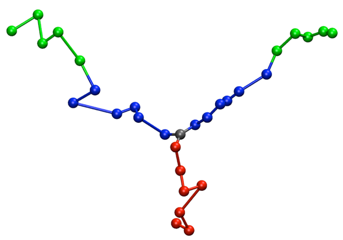
Shear cell setup



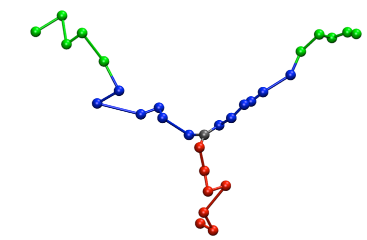


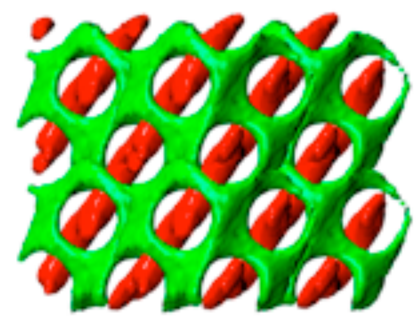
In situ shear small-angle neutron data
SANS-2, Paul Scherrer Institute

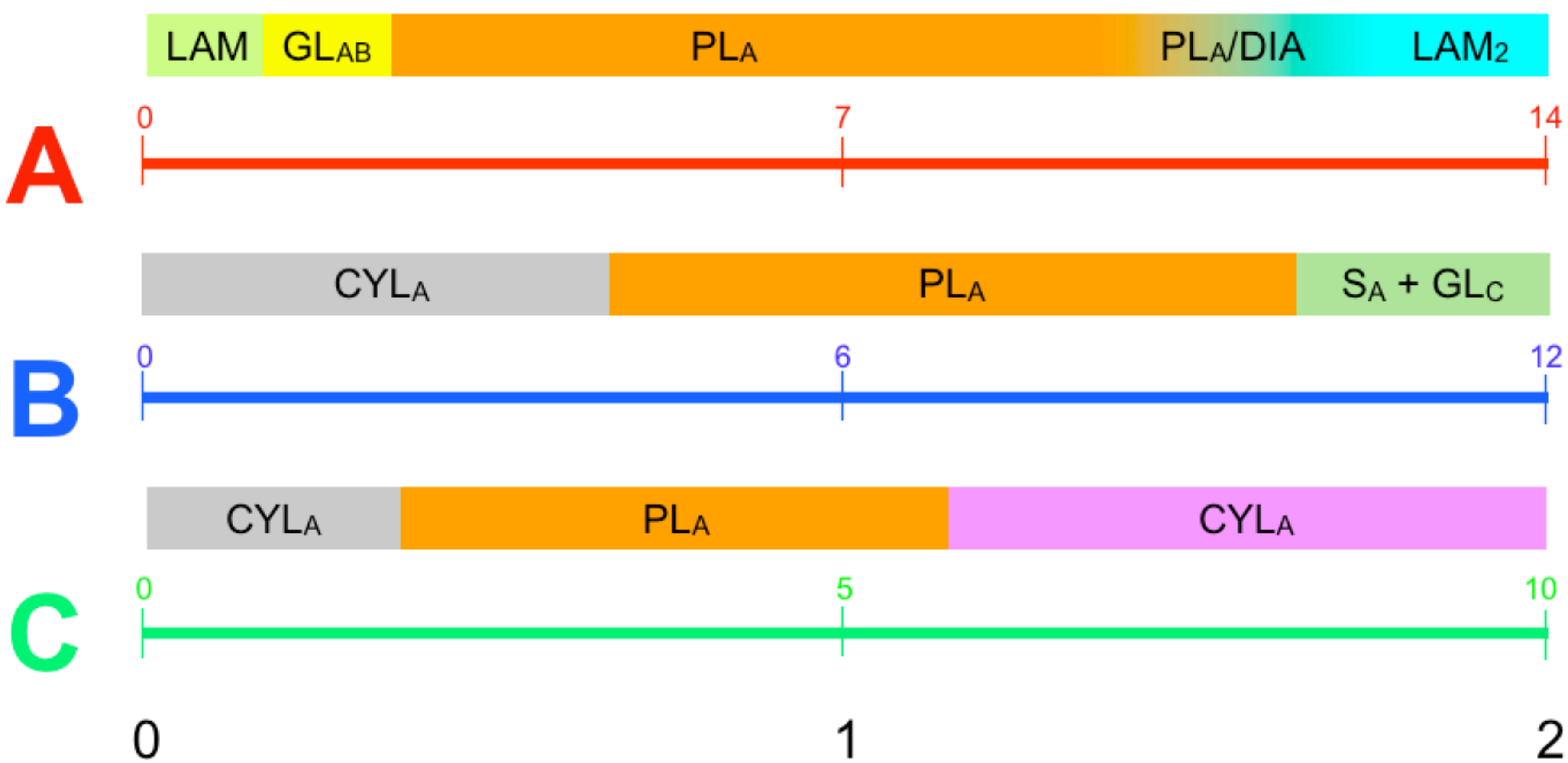
Simulations: Kirkensgaard JJK, *Soft Matter*, 2010, 6, 6102-6108
Experimental: Kirkensgaard JJK, Fragouli P, Hadjichristidis N and Mortensen K *Macromolecules*, 2011, 44 (3), 575-582



Phase diagram







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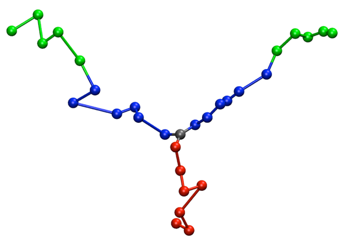
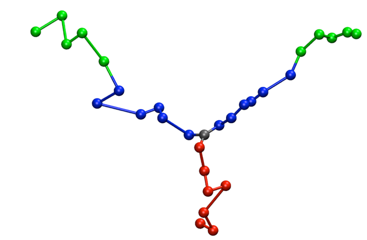
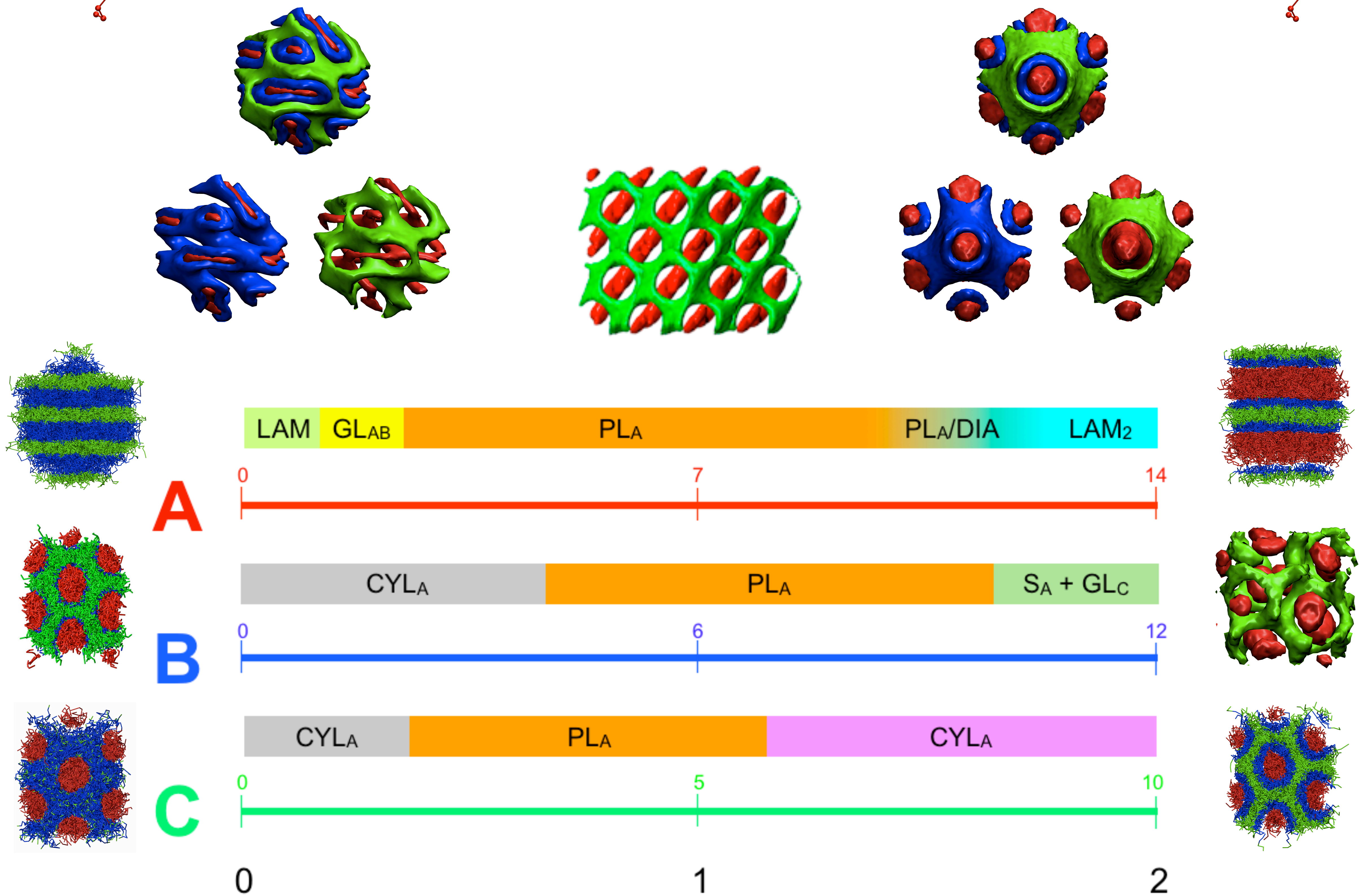
Experimental: Kirkensgaard JJK, Fragouli P, Hadjichristidis N and Mortensen K *Macromolecules*, 2011, 44 (3), 575-582



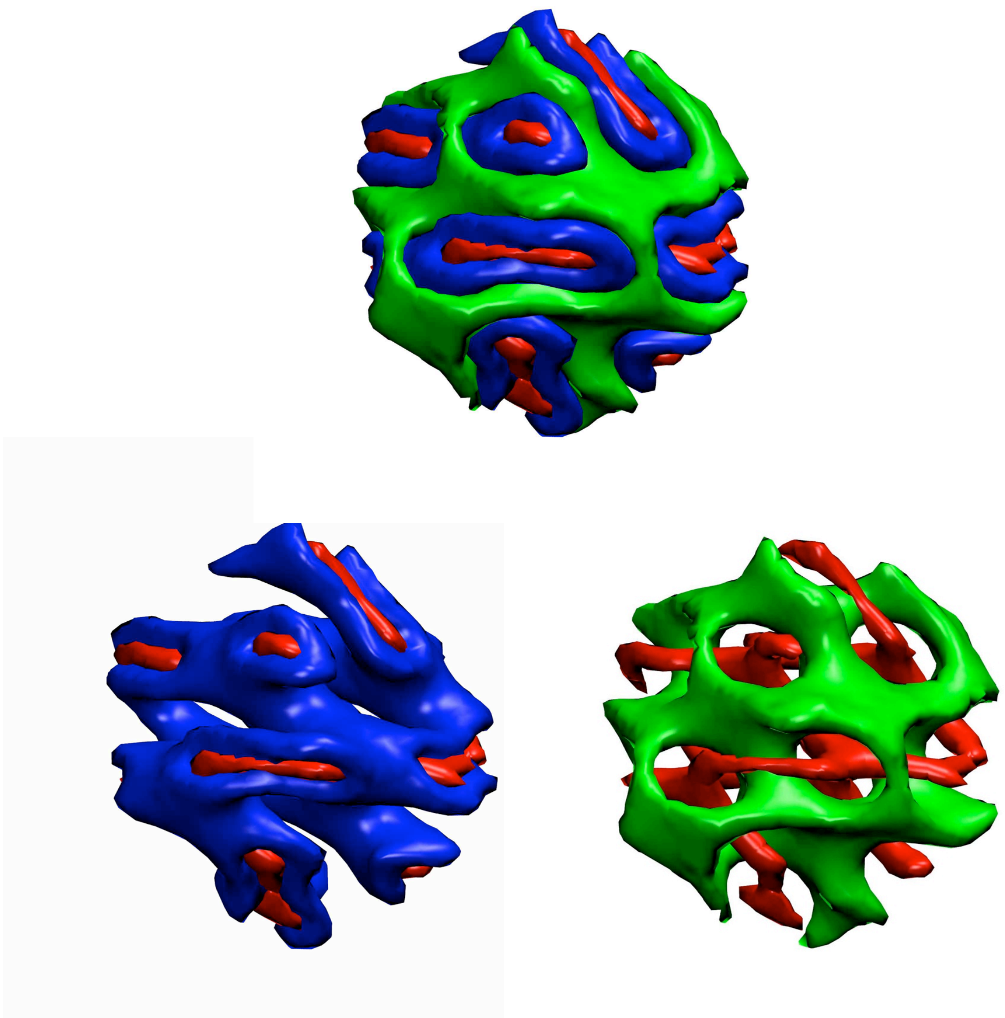
A(BC)$_2$ 3-miktoarm

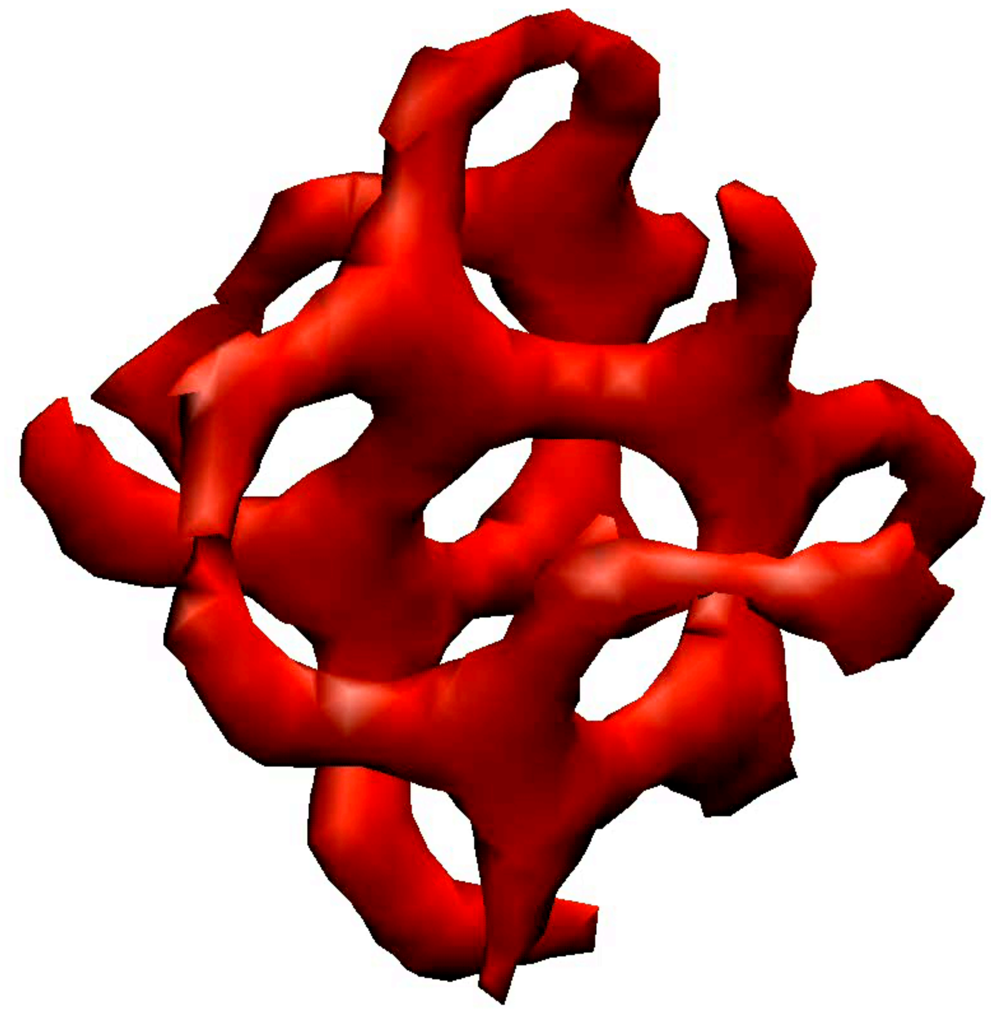




Simulations: Kirkensgaard JJK, *Soft Matter*, 2010, 6, 6102-6108
Experimental: Kirkensgaard JJK, Fragouli P, Hadjichristidis N and Mortensen K *Macromolecules*, 2011, 44 (3), 575-582

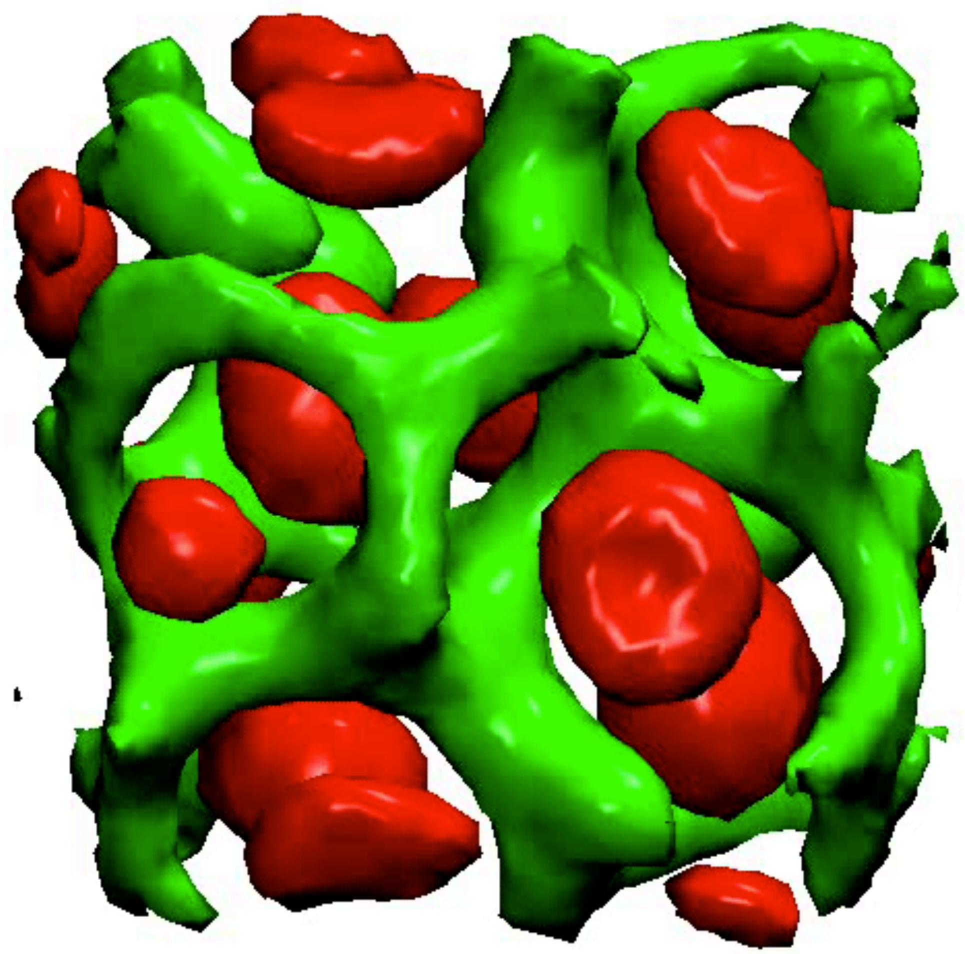
[GL$_{AB}$] - single network core-shell structure





Structure from A1-(B3-C3)$_2$ molecule

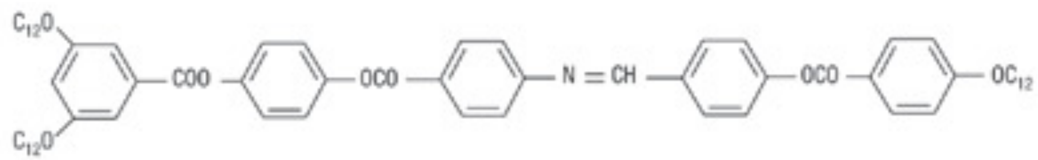
[S_A + GL_C] - sphere packing and single network



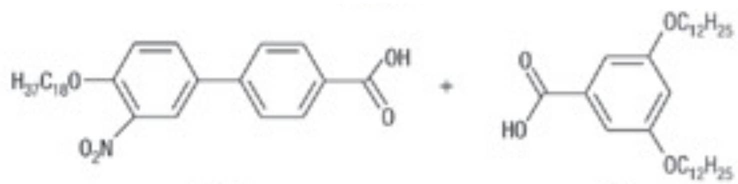
Structure from A4-(B9-C3)$_2$ molecule

Tricontinuous structures in ABC star systems?

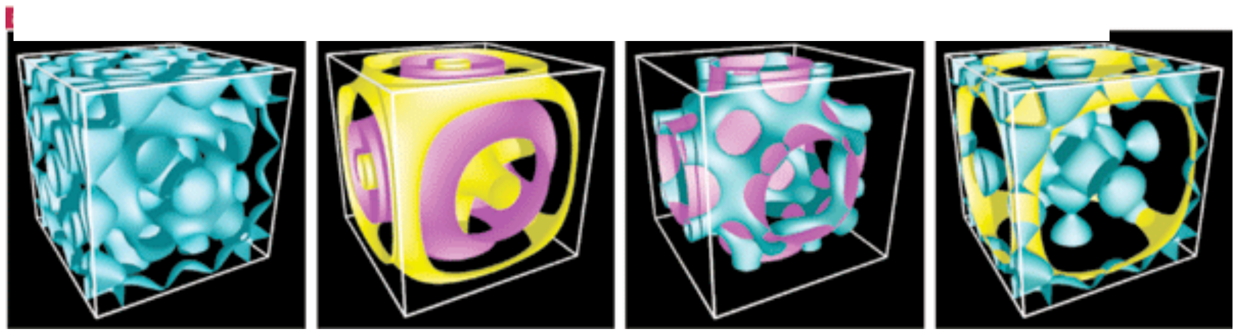
Asymmetric mesogen

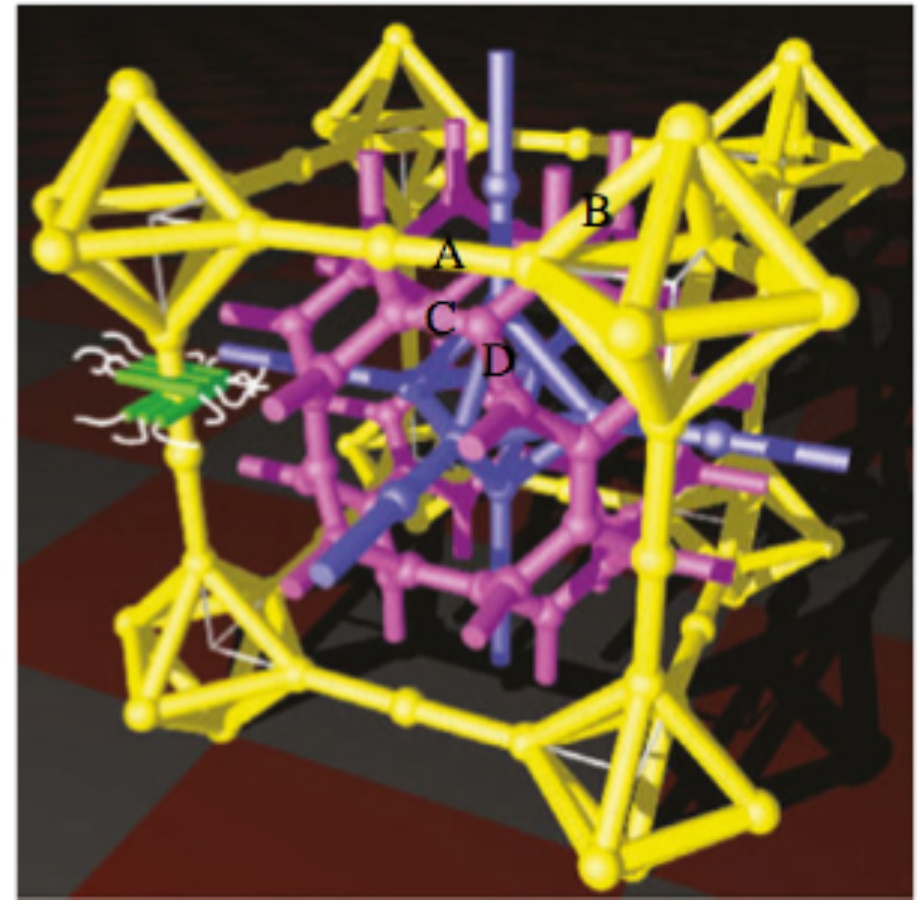


MIxture of carboxylic acids



90% 10%





Zeng et al, Nature Materials, 4, 2005

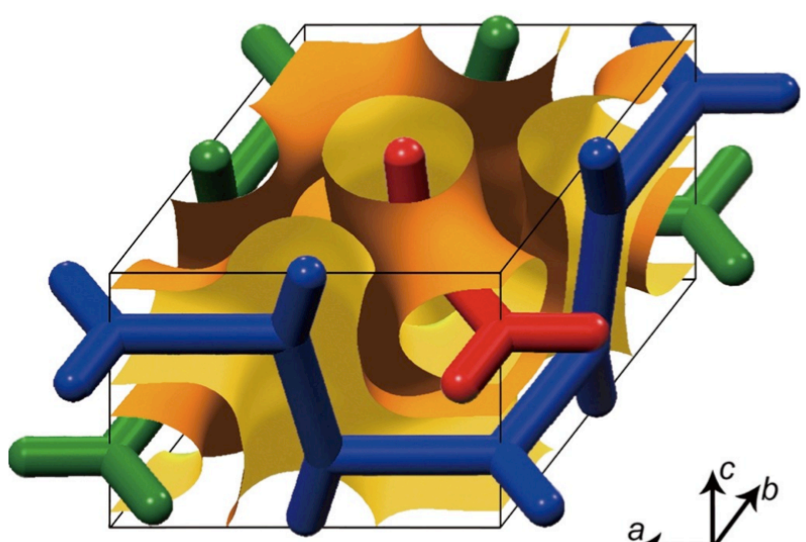
nature chemistry ARTICLES
PUBLISHED ONLINE: 6 APRIL 2009 | DOI: 10.1038/NCHEM.166

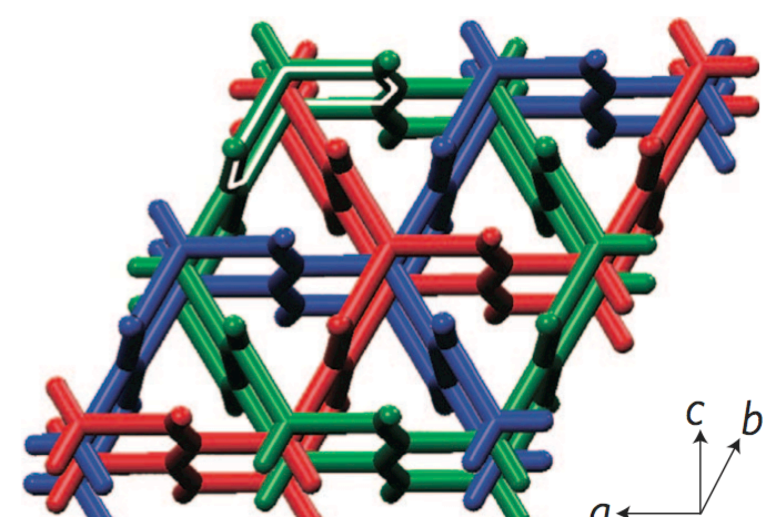
A tri-continuous mesoporous material with a silica pore wall following a hexagonal minimal surface

Yu Han[1†‡], Daliang Zhang[2,3‡], Leng Leng Chng[1], Junliang Sun[2], Lan Zhao[1], Xiaodong Zou[2*] and Jackie Y. Ying[1*]

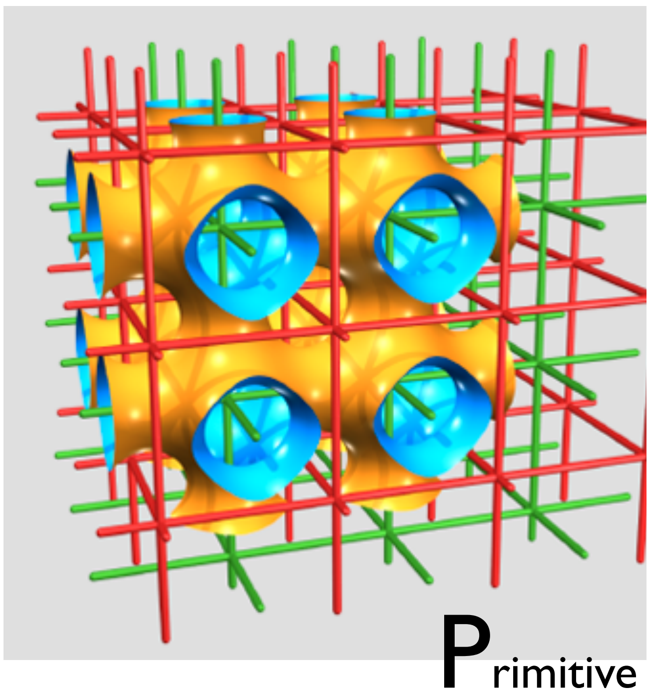
Han et al, Nature Chemistry, 1, 2009

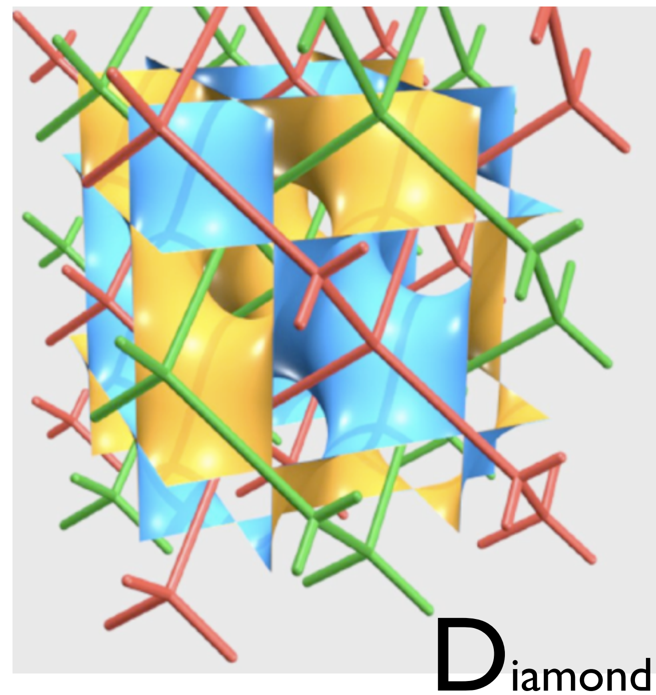
Also found in a surfactant system Soft Matter, 2014, 10, 8229

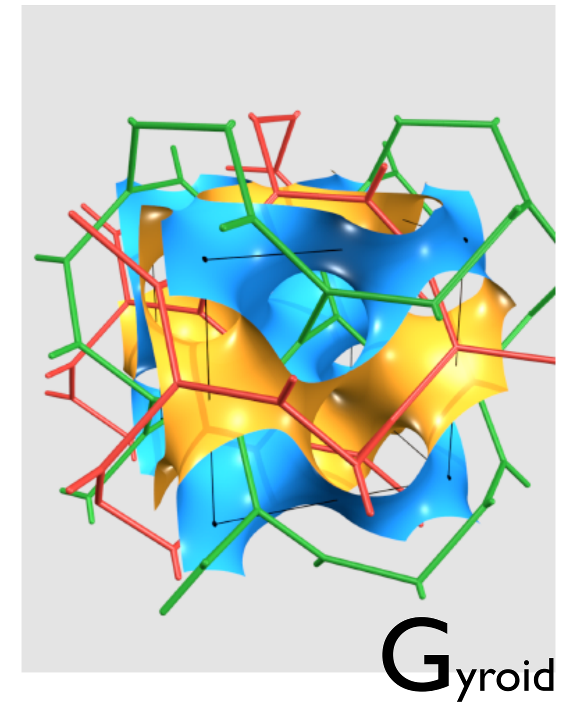


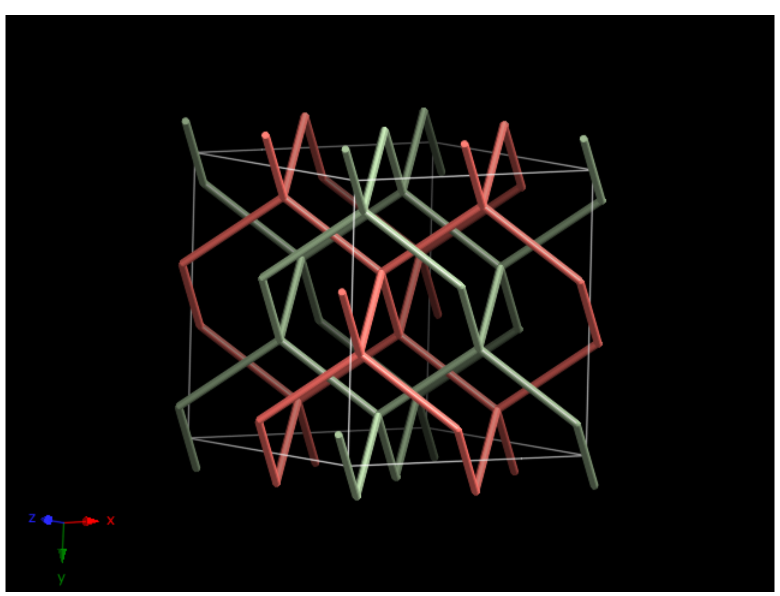


Construction of bicontinuous patterns

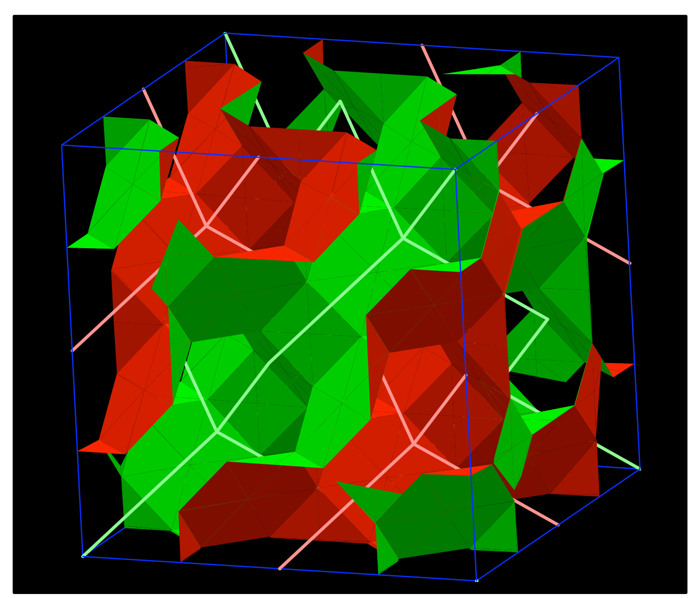




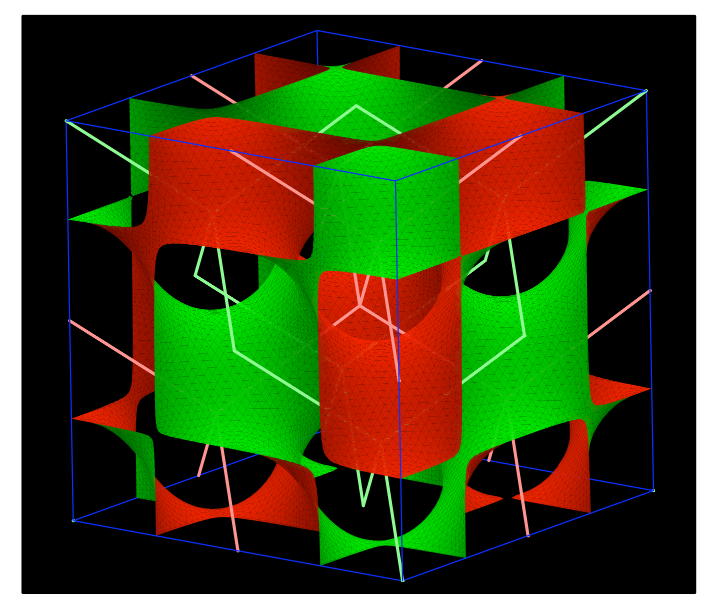




Take two threaded nets,
here double diamond



Construct Voronoi partition
of net nodes

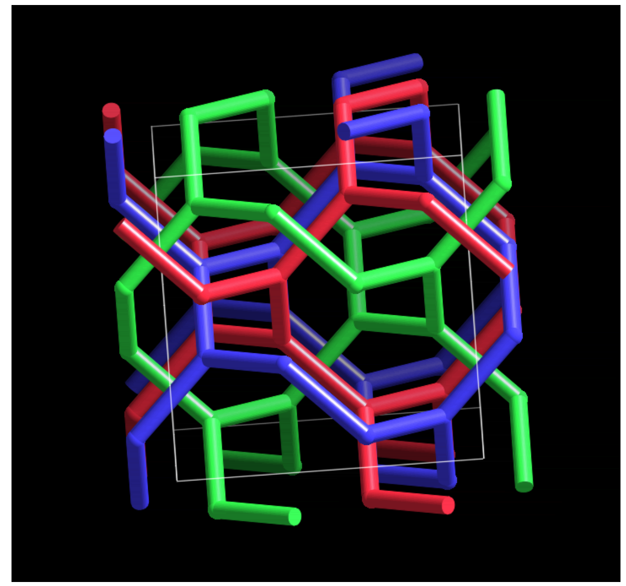


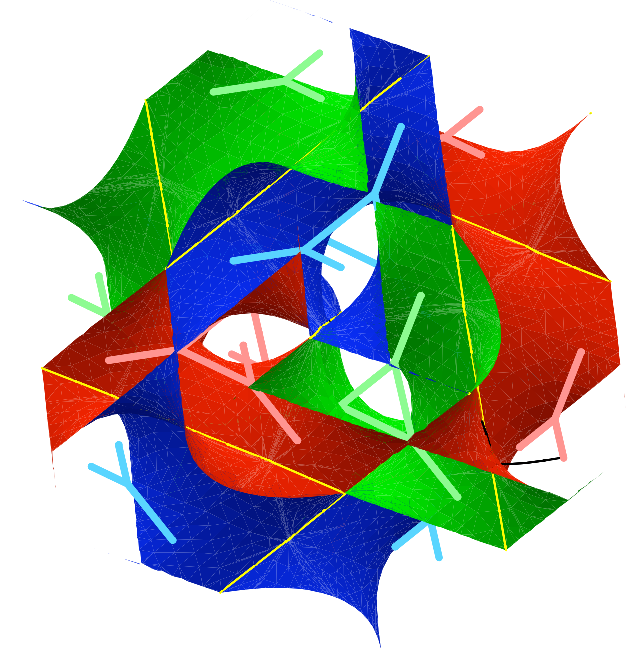
Minimize area of Voronoi walls
with K. Brakke's *Surface Evolver*

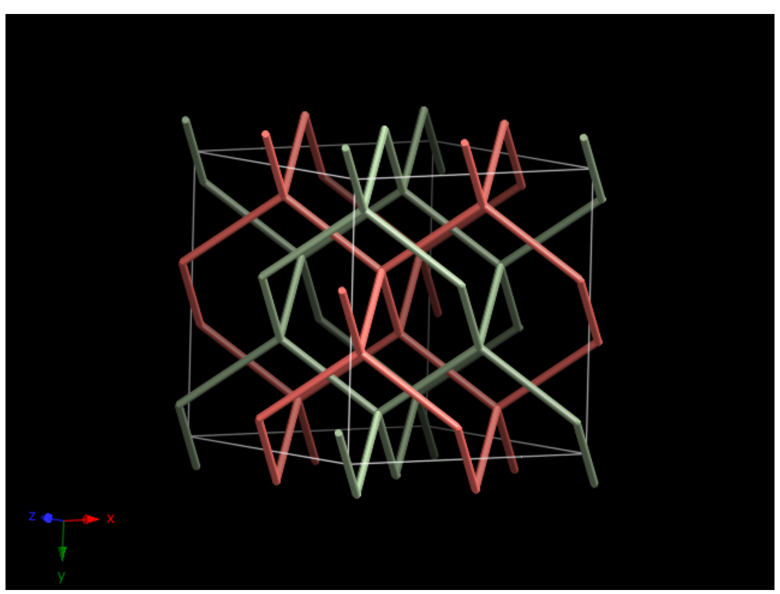
Construction of tricontinuous patterns

Do the same with 3 nets!
Here triple gyroid (3srs).

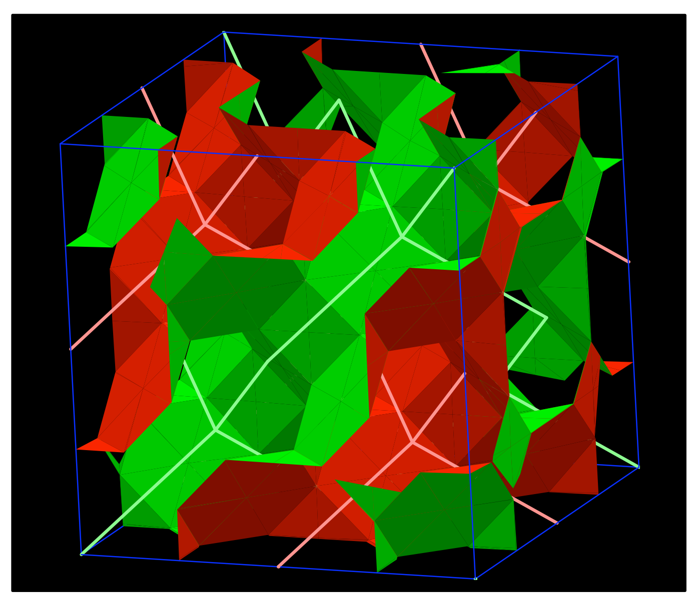
MANY polycontinuous patterns are possible! We are only interested in those with unbranched junction lines.



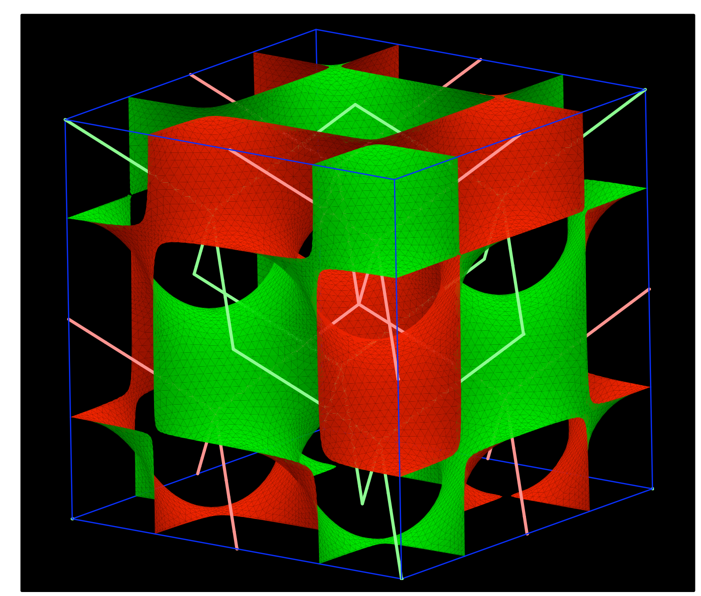




Take two threaded nets, here double diamond

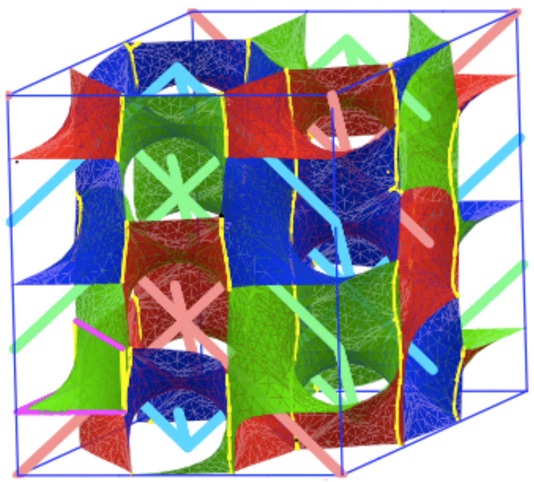


Construct Voronoi partition of net nodes

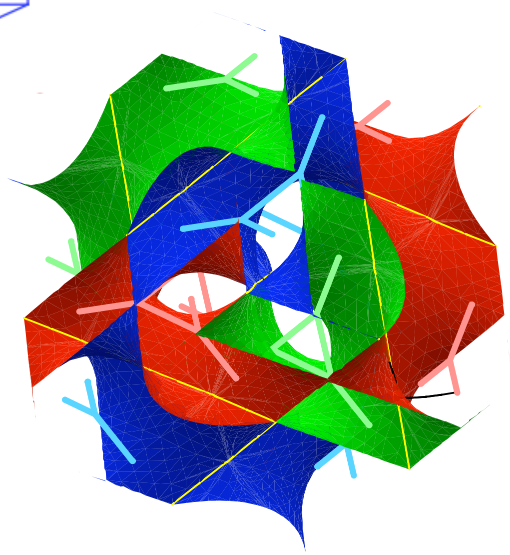


Minimize area of Voronoi walls with K. Brakke's *Surface Evolver*

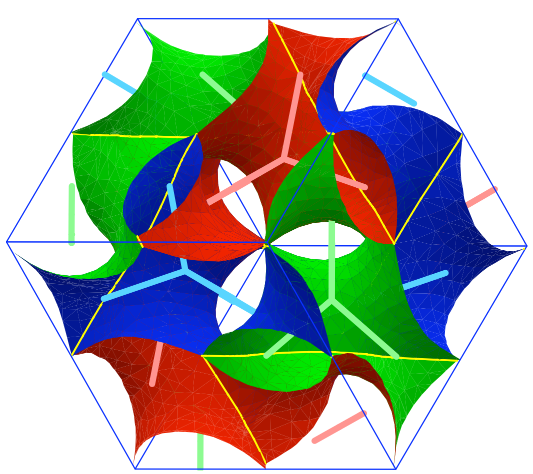
Some possible tricontinuous patterns



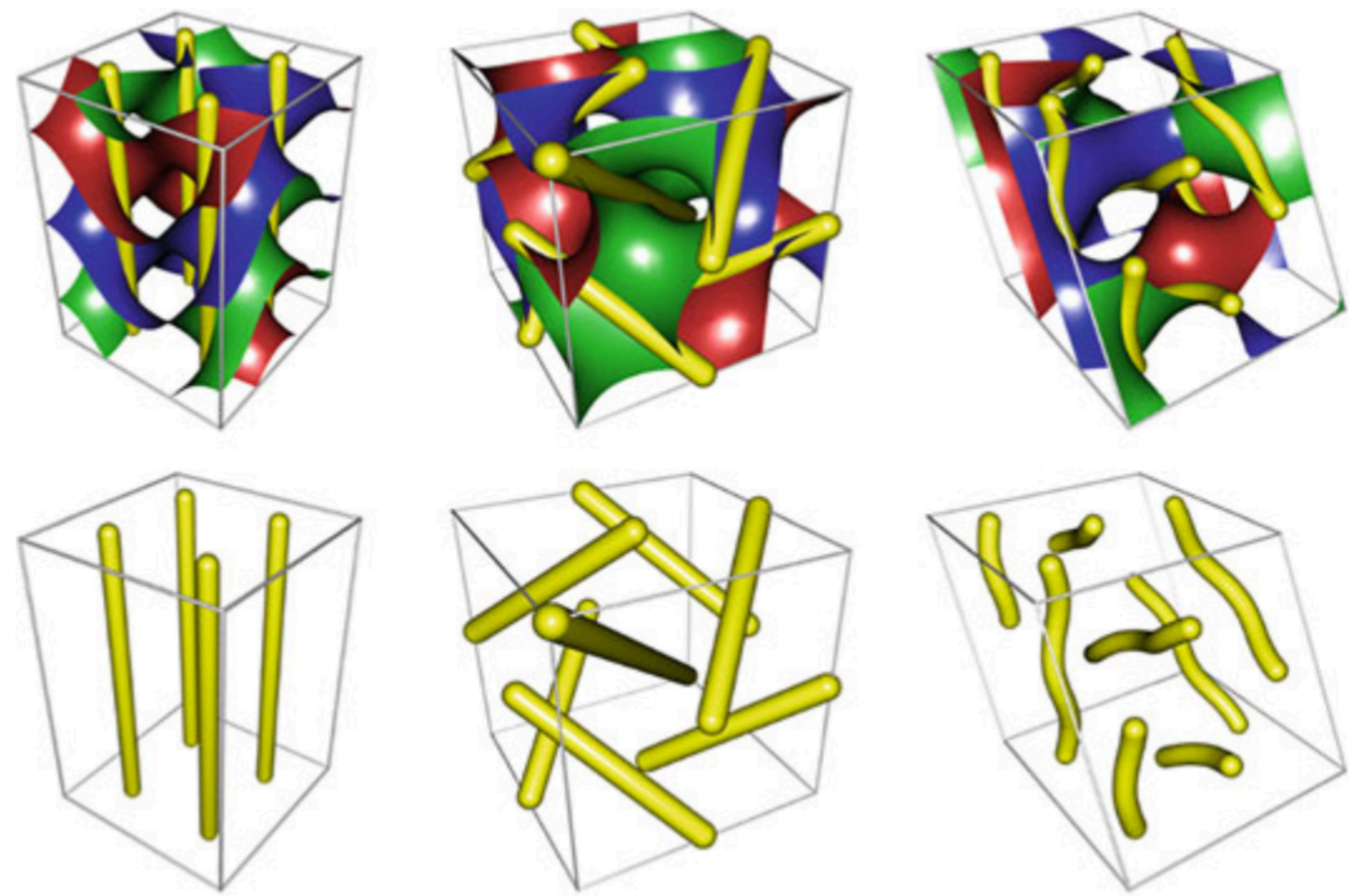
Triple P (3pcu)



Triple G (3srs)



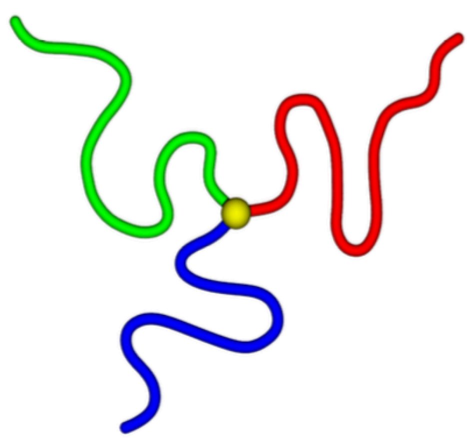
Triple D (3dia)

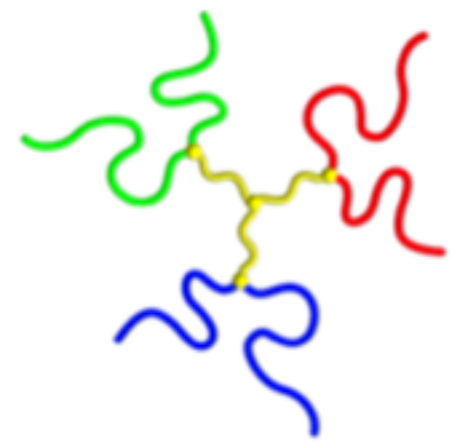


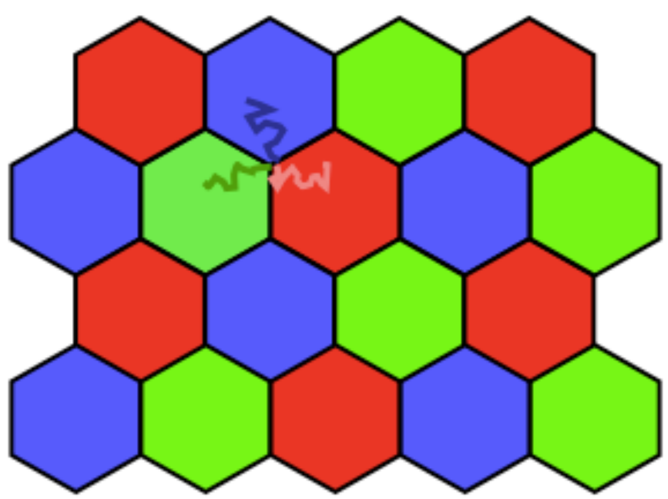
(a) 3dia(109) (b) 3srs(24) (c) 3qtz(145)

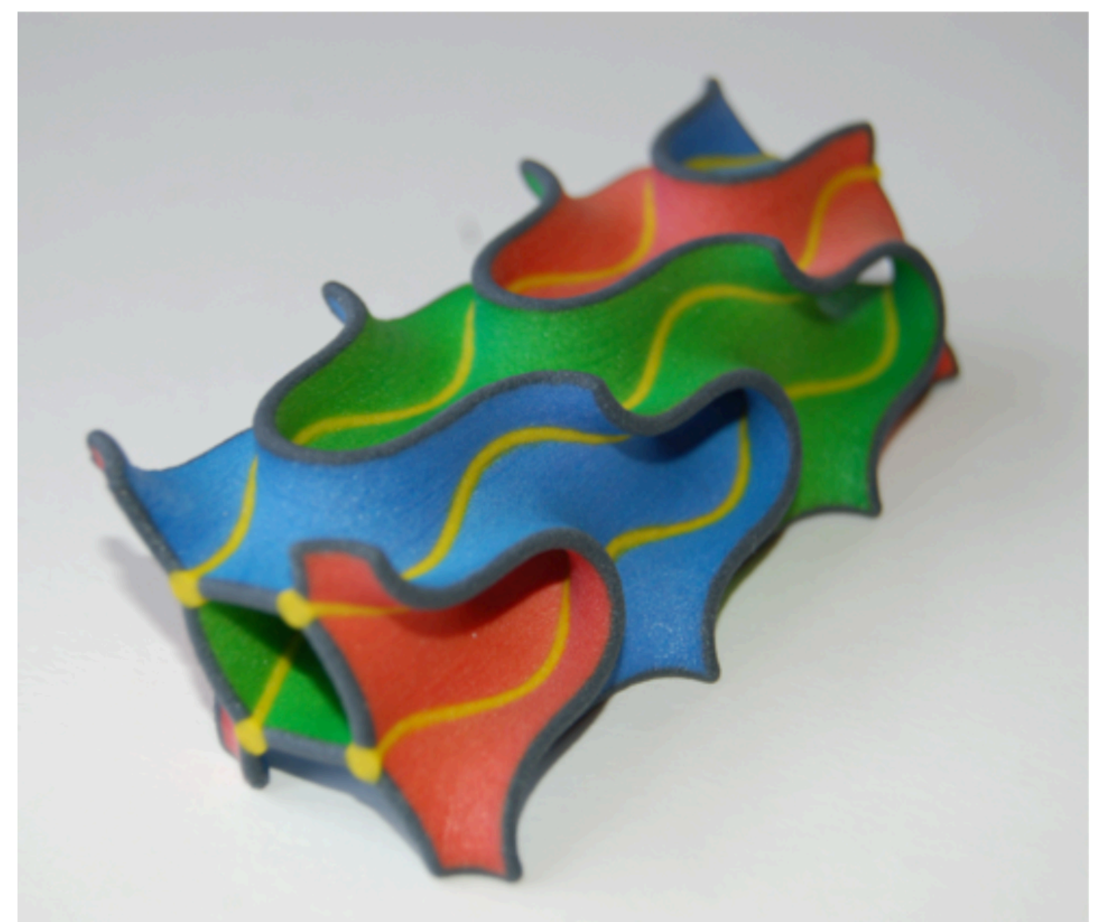
Hyde, de Campo, Oguey, Soft Matter, 2009
Fischer, de Campo, Kirkensgaard, Hyde and Schröder-Turk, Macromolecules, 47, 2014

Tricontinuous 3-colored structures



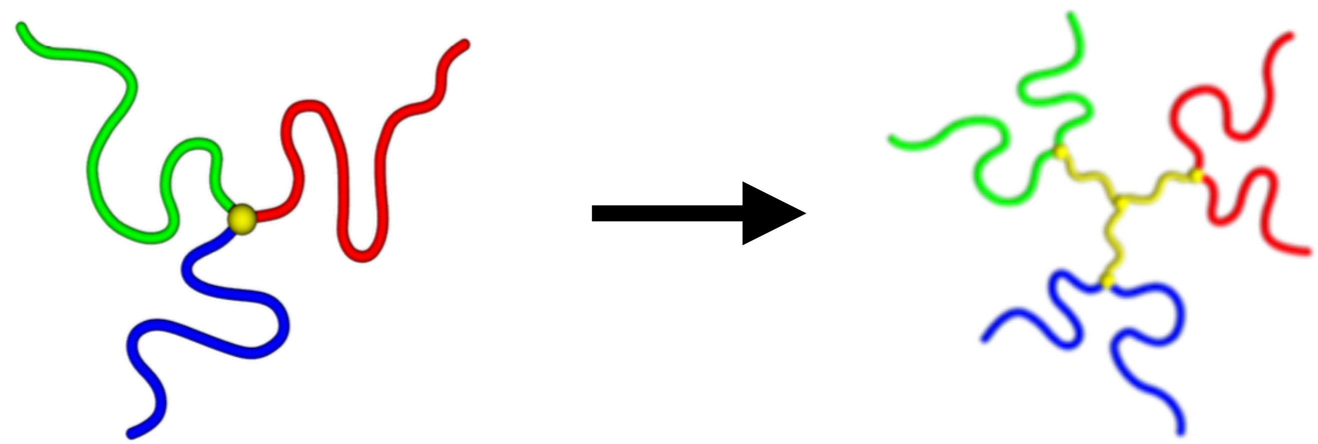


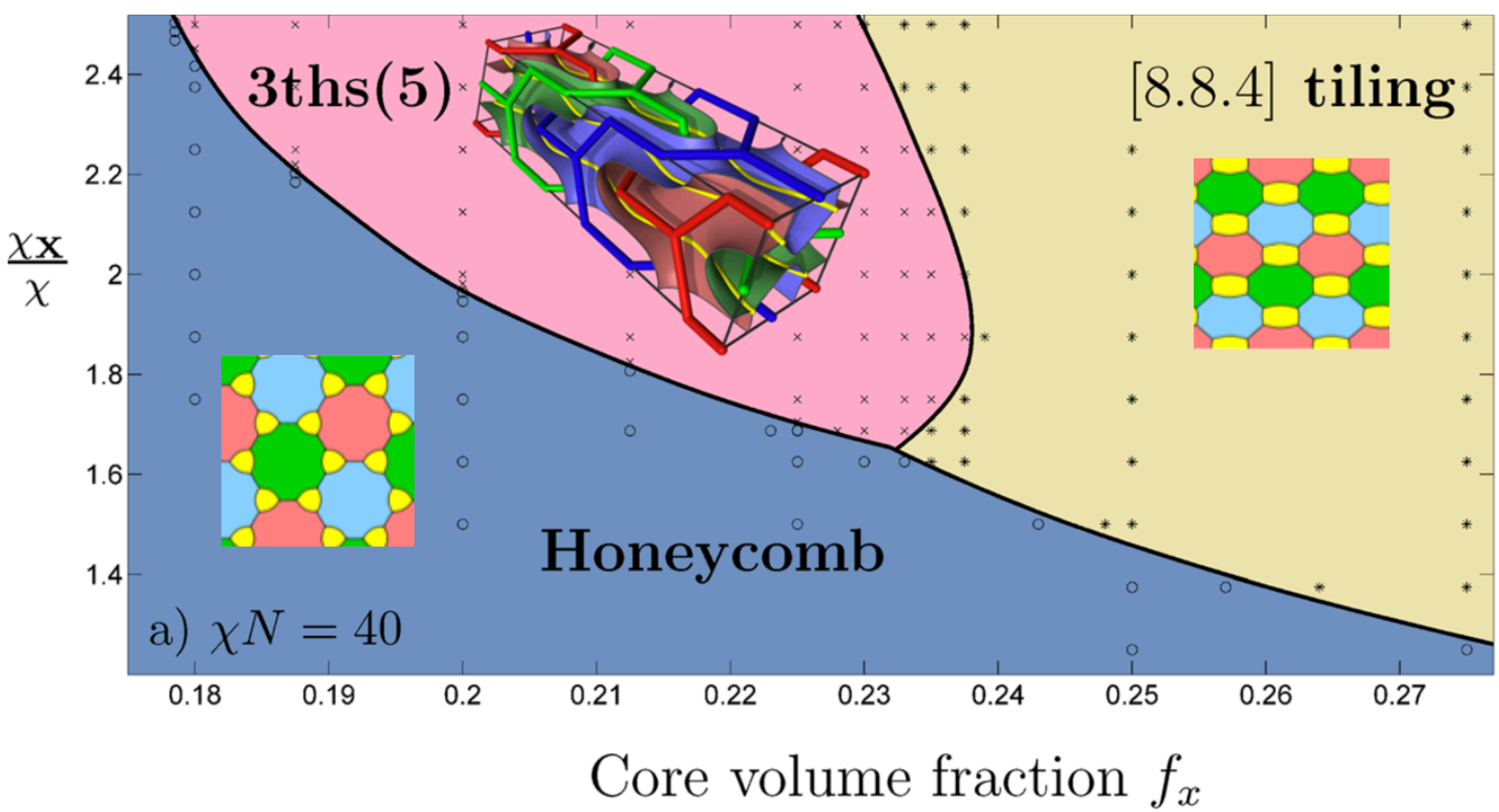




Fischer, de Campo, Kirkensgaard, Hyde and Schröder-Turk, Macromolecules, 47, 2014

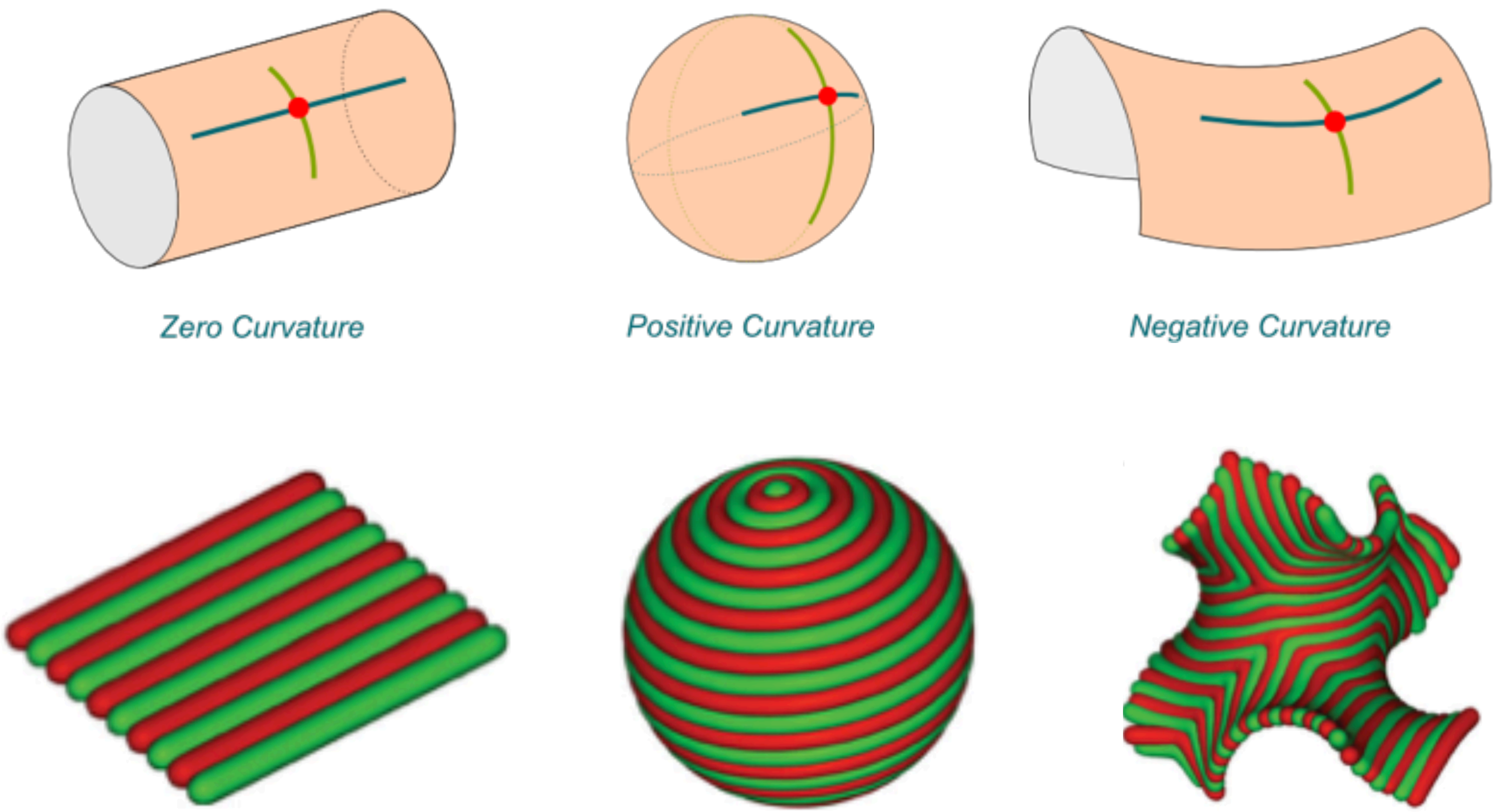
Tricontinuous 3-colored structures





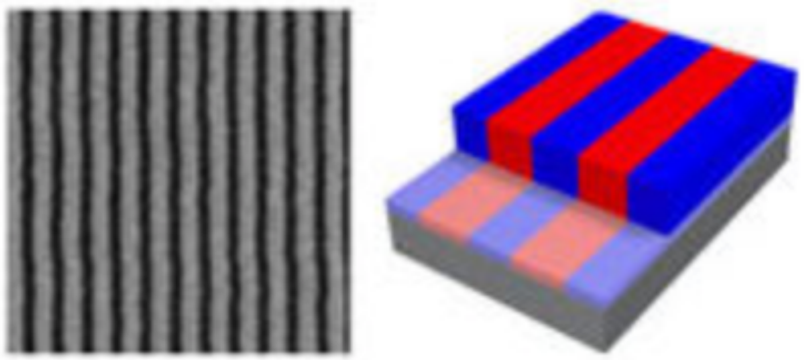
Fischer, de Campo, Kirkensgaard, Hyde and Schröder-Turk, Macromolecules, 47, 2014

From flat to curved space

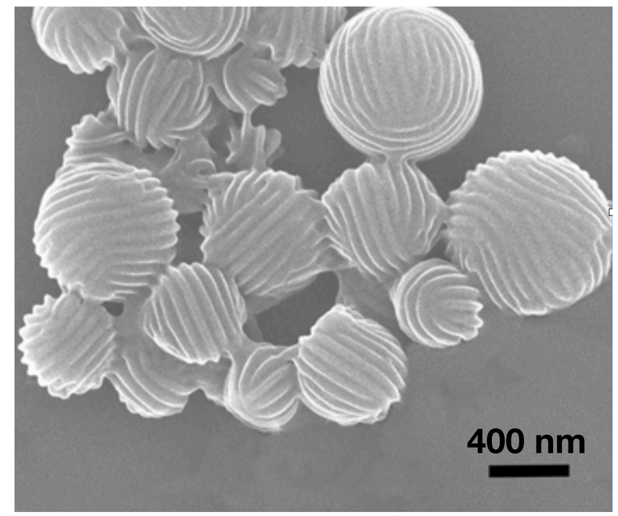


Images from Interface Focus 7: 20160130 (2017) and http://www.science4all.org/article/brazuca/

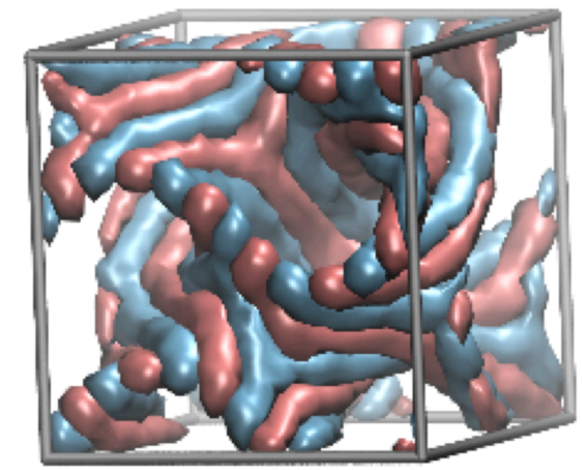
From flat to curved space



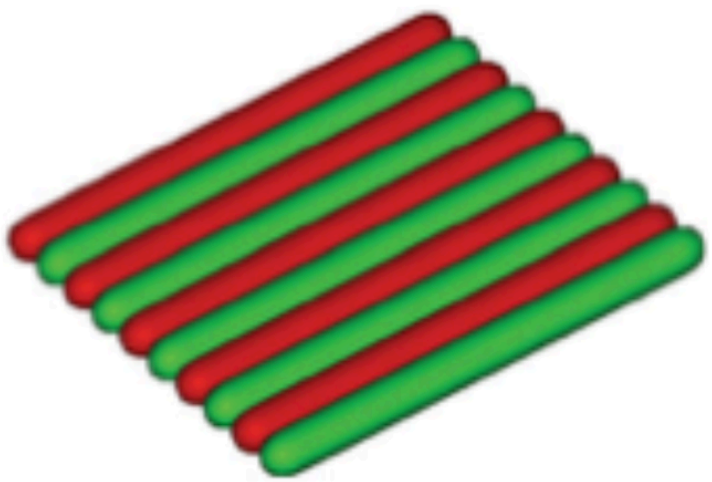
BCP’s on templated substrate
Nature Communications 7, 12366 (2016)

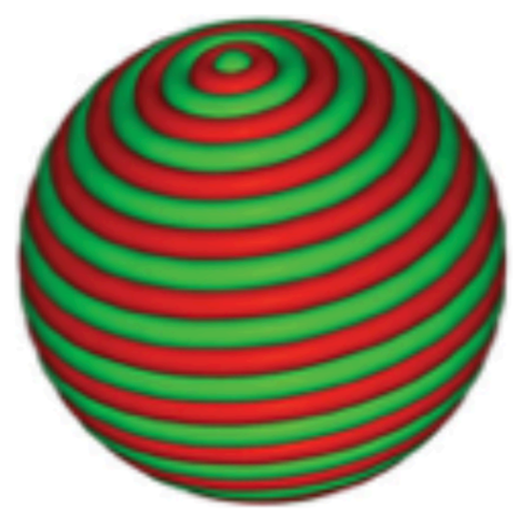


BCP striped nano spheres
Scientific Reports | 6:29796 (2016)



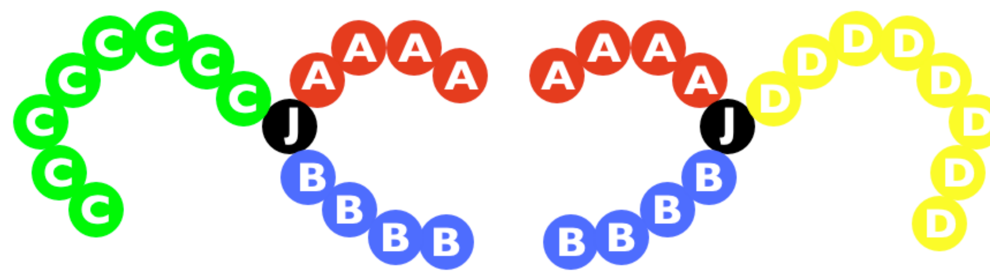
BCP 3-armed stars minority components
PNAS, 111, 4, 1271 (2015)





Images from Interface Focus 7: 20160130 (2017) and http://www.science4all.org/article/brazuca/

Blending ABC and ABD 3-miktoarm stars

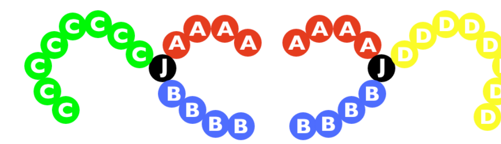


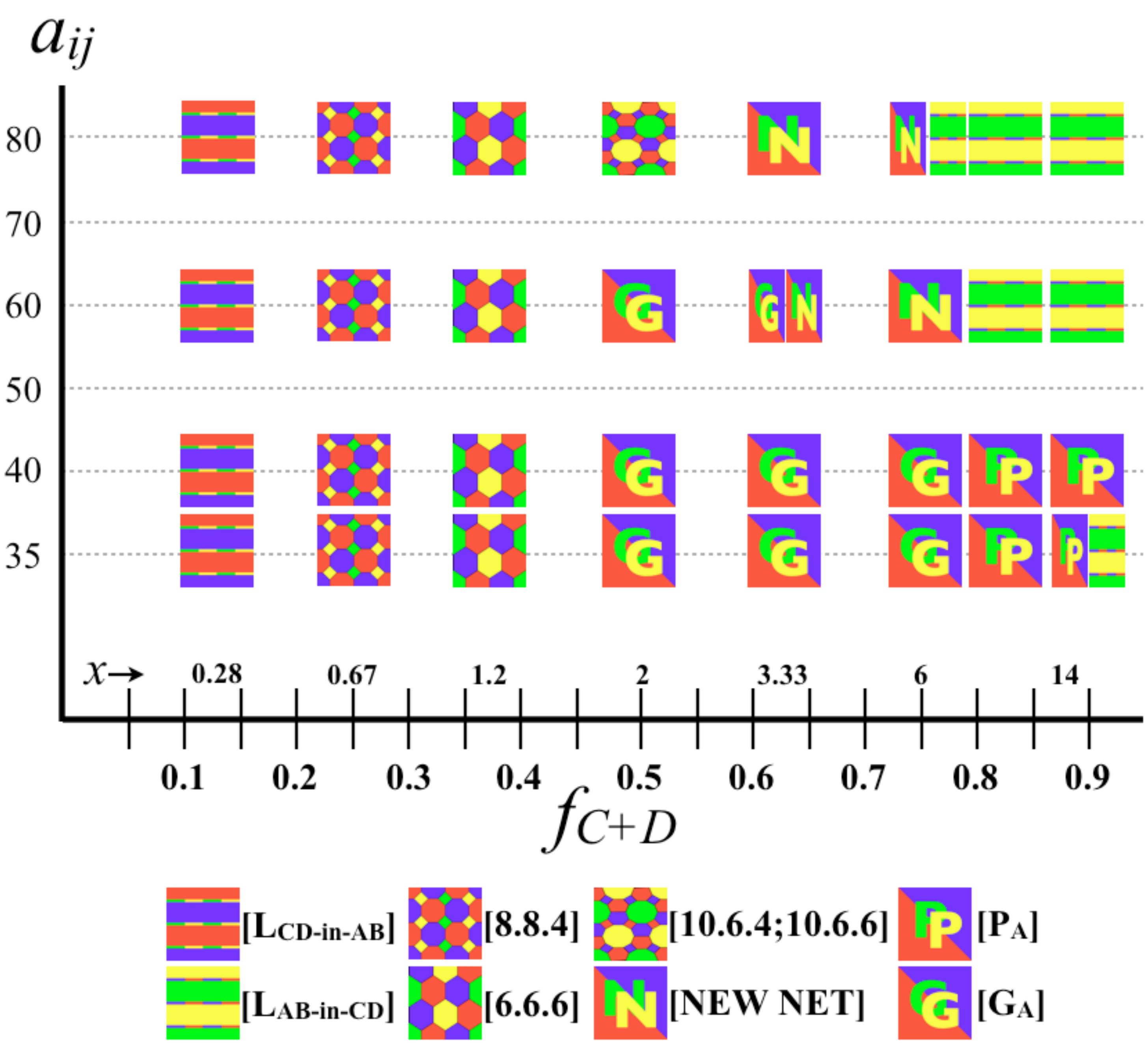
AB and CD constrained in
pairs to have the same size.

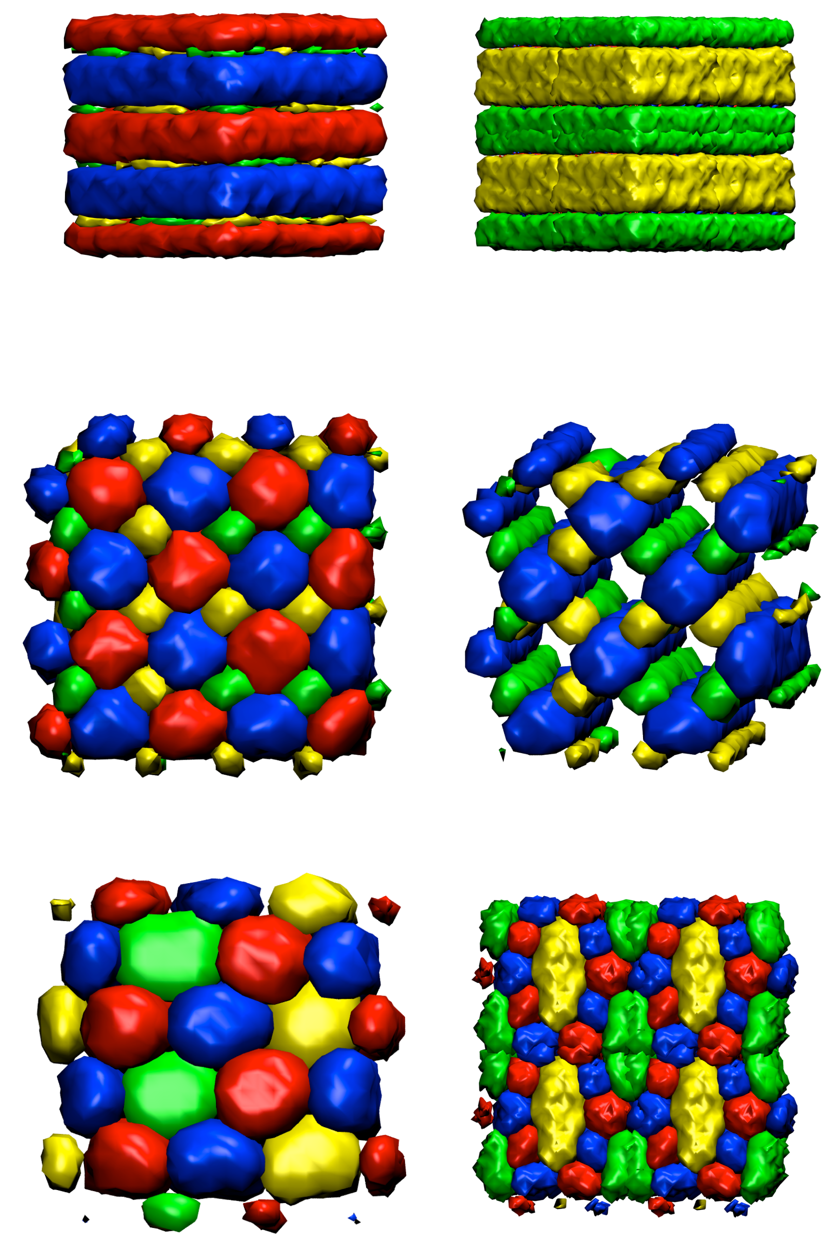
Again define ratio x = C/A to
compare with pure ABC stars.
Here x = 2.

Investigate at 4 segregation
levels - all symmetric.

Blending ABC and ABD 3-miktoarm stars







Kirkensgaard JJK, Interface Focus,2, 602-607 (2012)

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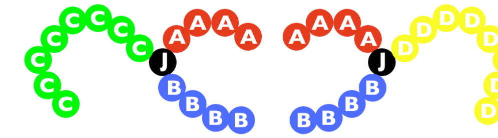

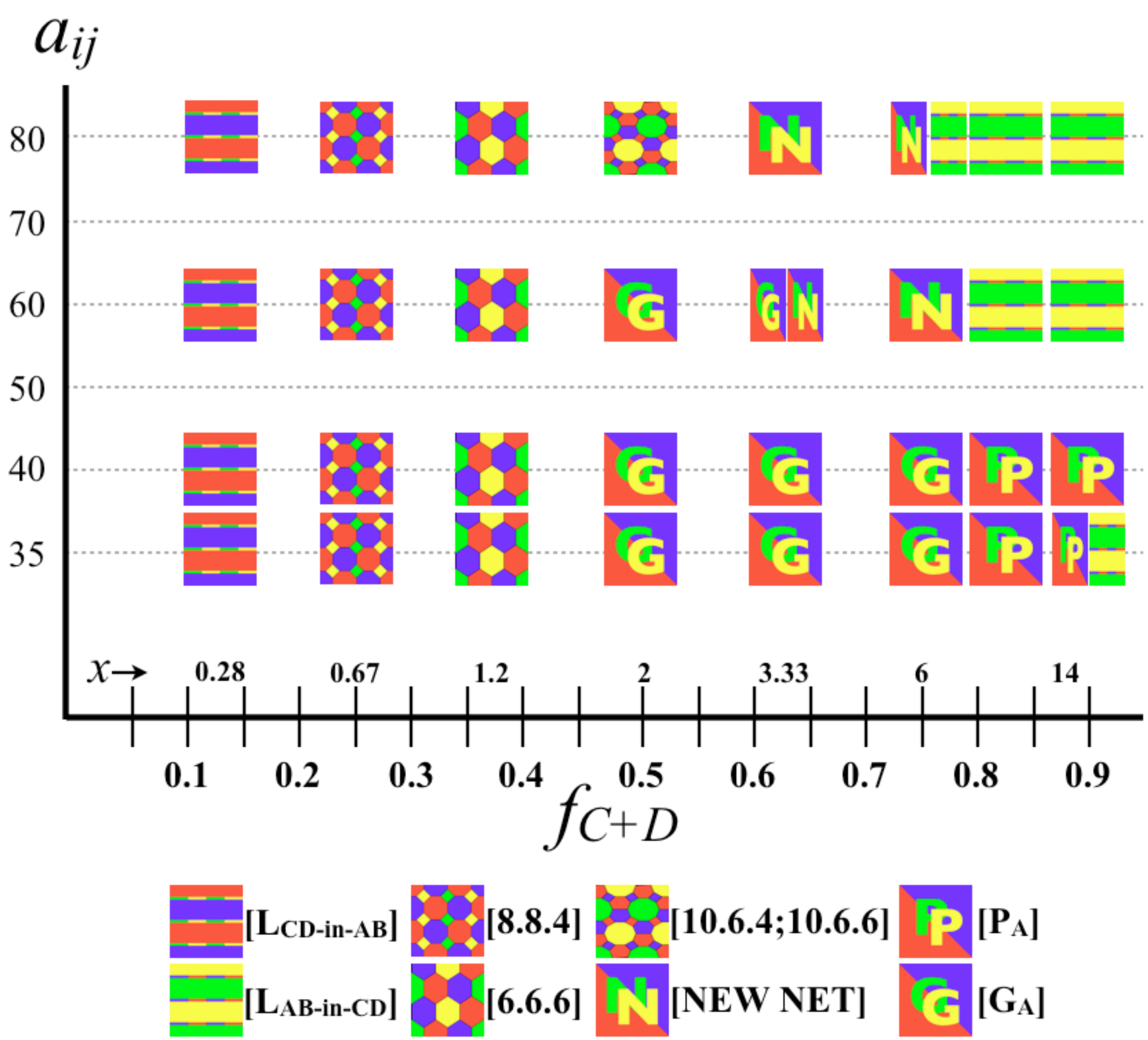

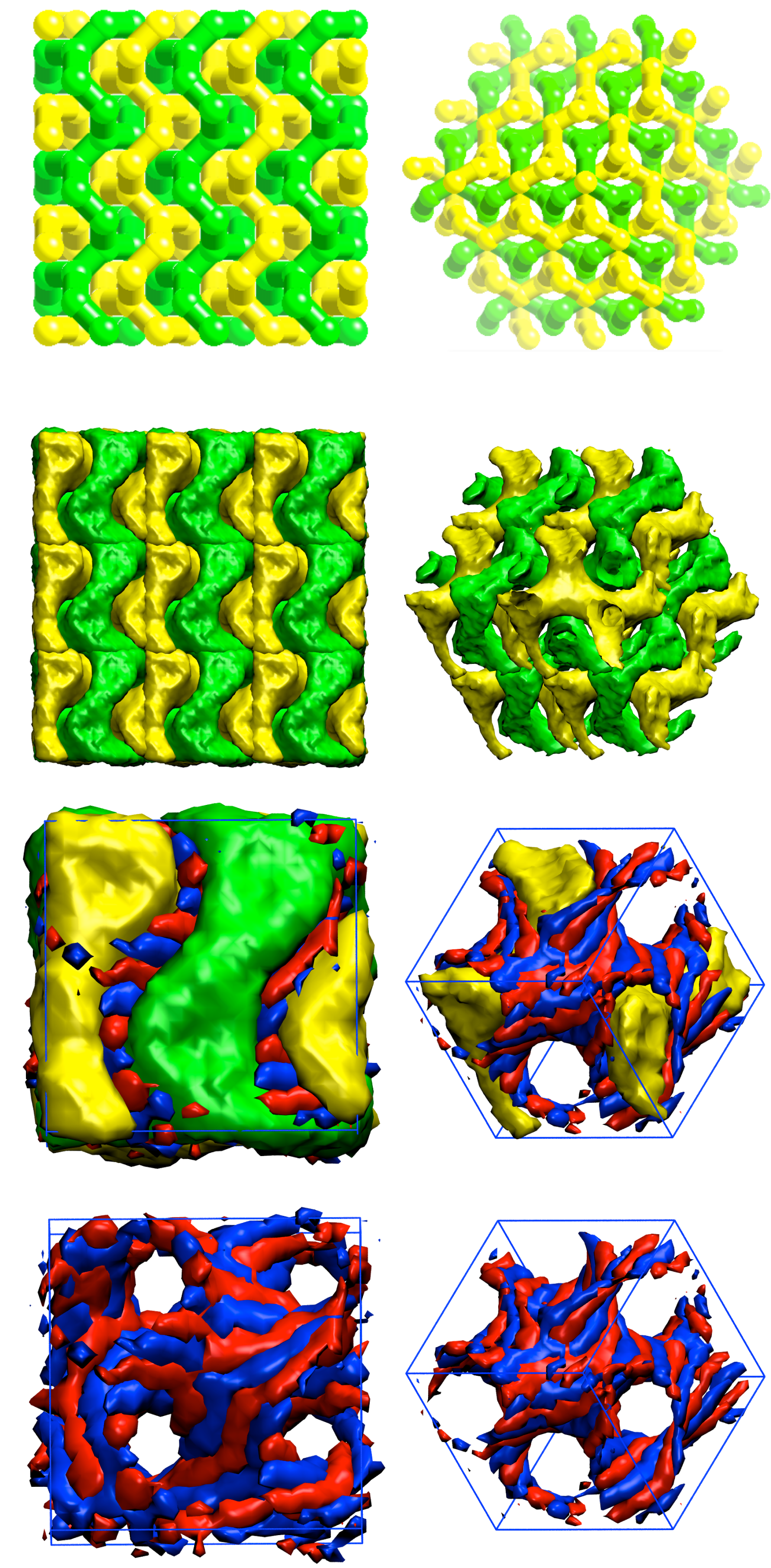

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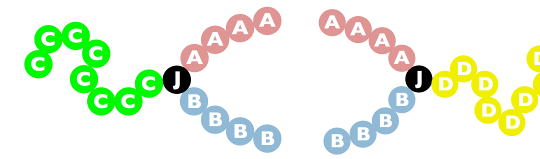
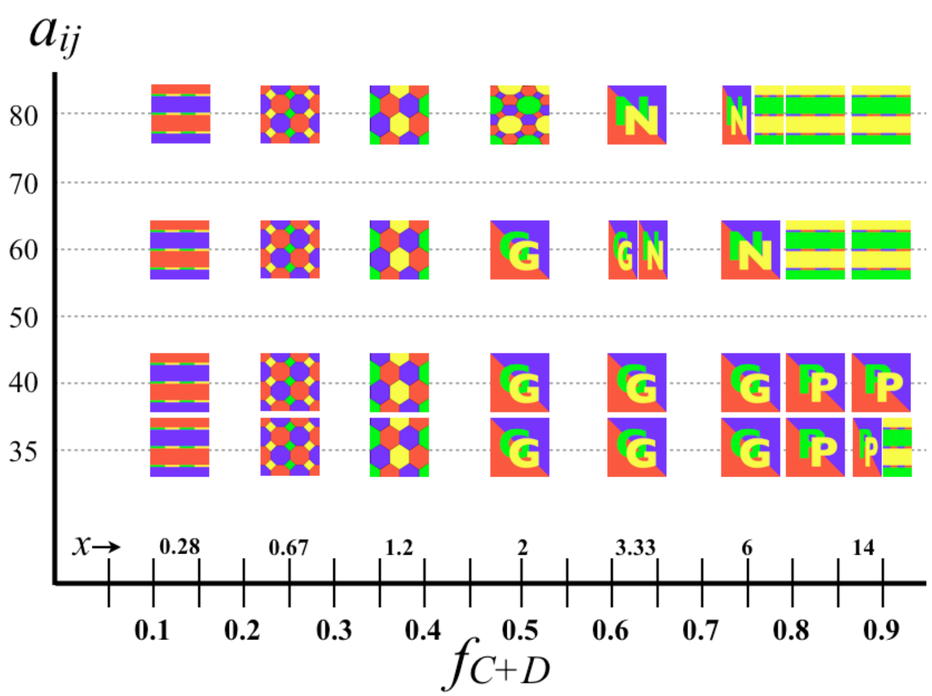
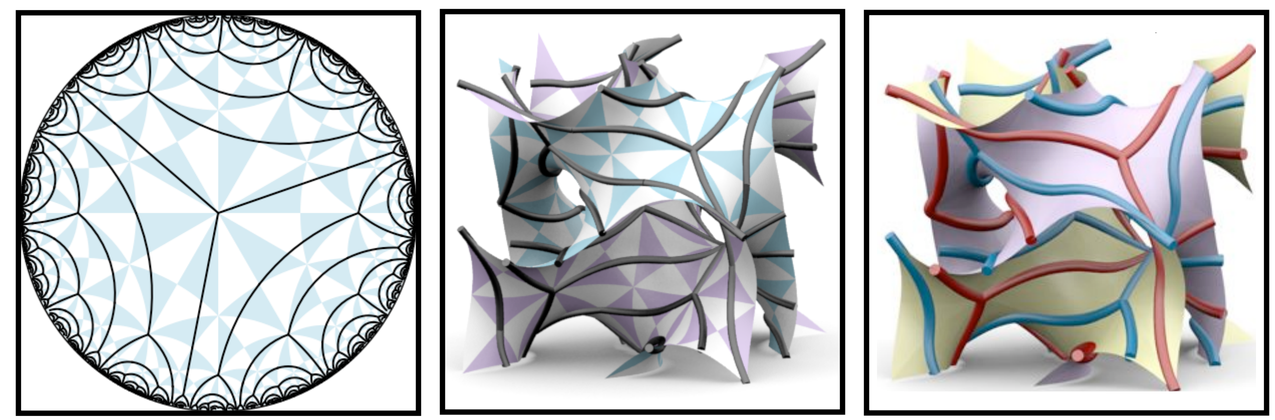
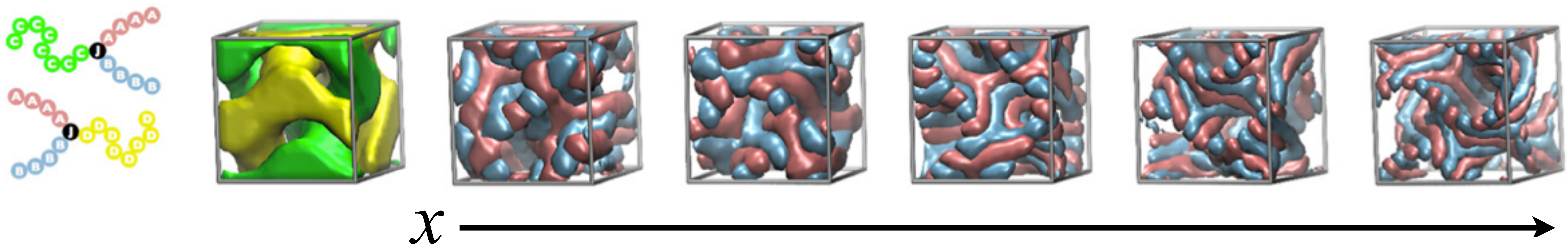
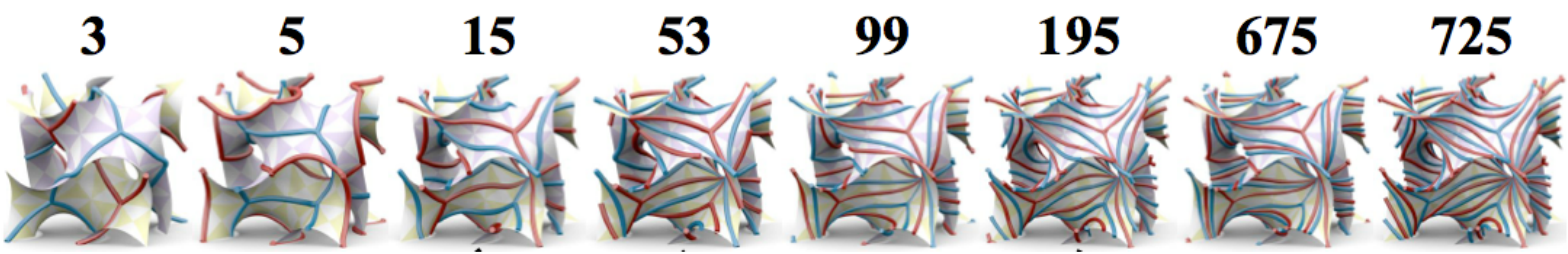










Kirkensgaard JJK, Evans ME, de Campo L and Hyde ST, PNAS, 111(4), 1271–1276 (2014)

Blending ABC and ABD 3-miktoarm stars

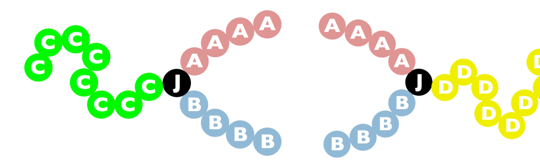
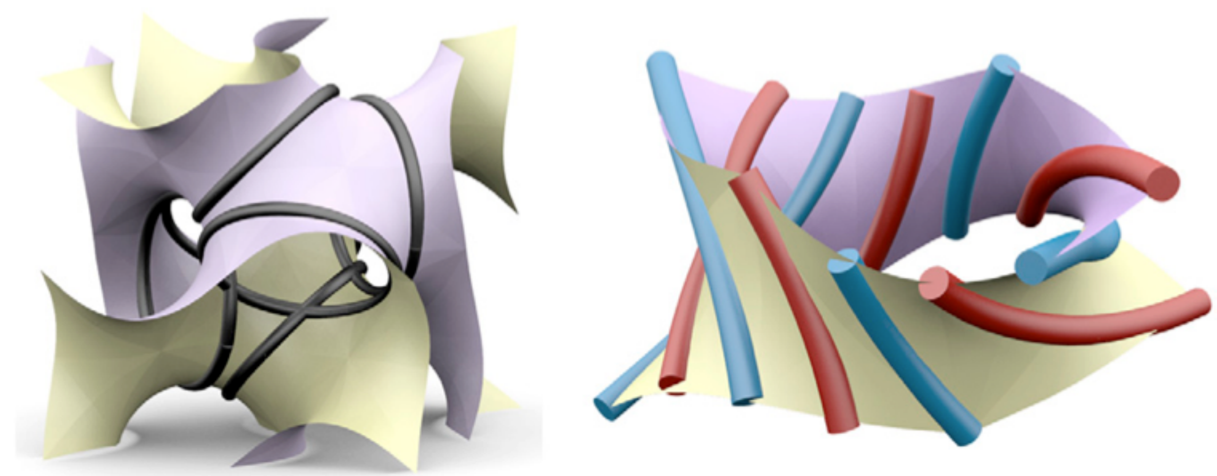
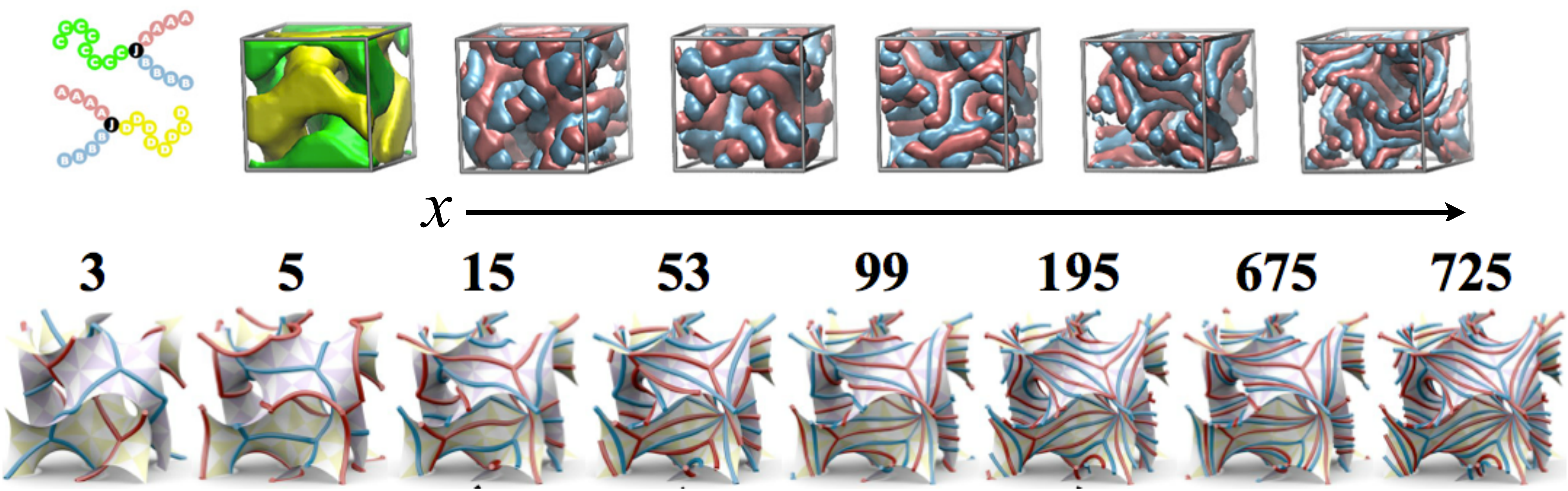


Table 1. Details of threaded multiple nets from regular dense hyperbolic forests mapped onto the Gyroid.

Tree edge length	# nets*	# stripes (i)†	# stripes (ii)†
$cosh^{-1}(3)$	2 srs	2	4
$cosh^{-1}(5)$	2 srs	2	6
$cosh^{-1}(15)$	4* hcb ‡	6	8
$cosh^{-1}(53)$	54 srs	10	10
$cosh^{-1}(99)$	54 srs	8	14
$cosh^{-1}(195)$	2 srs	12	14
$cosh^{-1}(675)$	54 srs	10	20
$cosh^{-1}(725)$	54 srs	14	18





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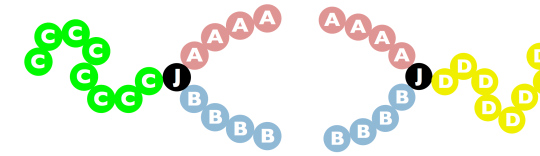

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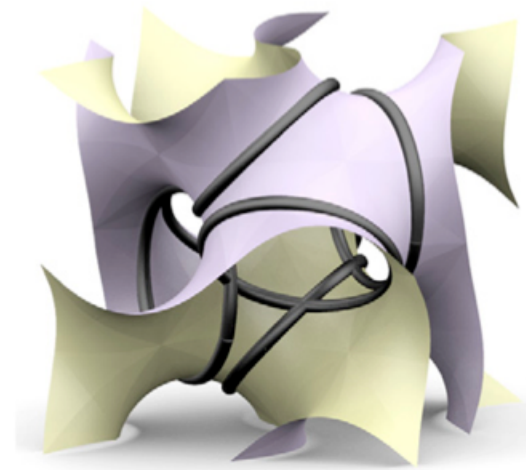
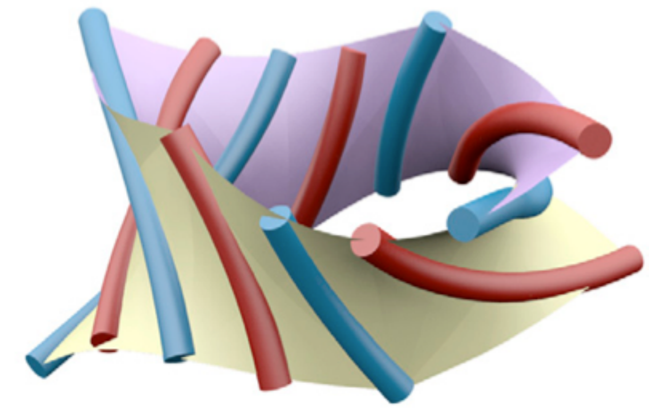
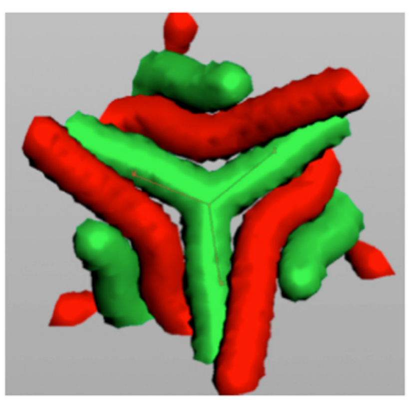
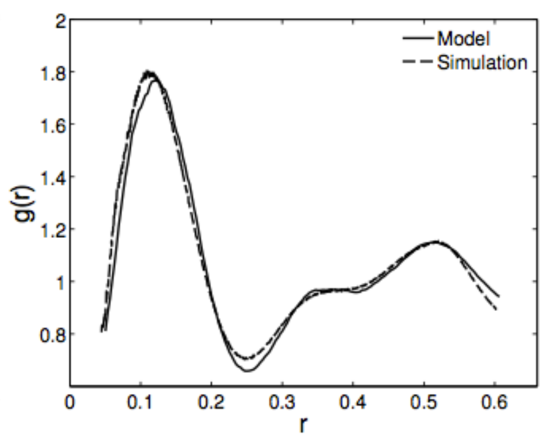
$\cosh^{-1}(15)$	4* **hcb** ‡	6	8
$\cosh^{-1}(53)$	54 **srs**	10	10
$\cosh^{-1}(99)$	54 **srs**	8	14
$\cosh^{-1}(195)$	2 **srs**	12	14
$\cosh^{-1}(675)$	54 **srs**	10	20
$\cosh^{-1}(725)$	54 **srs**	14	18

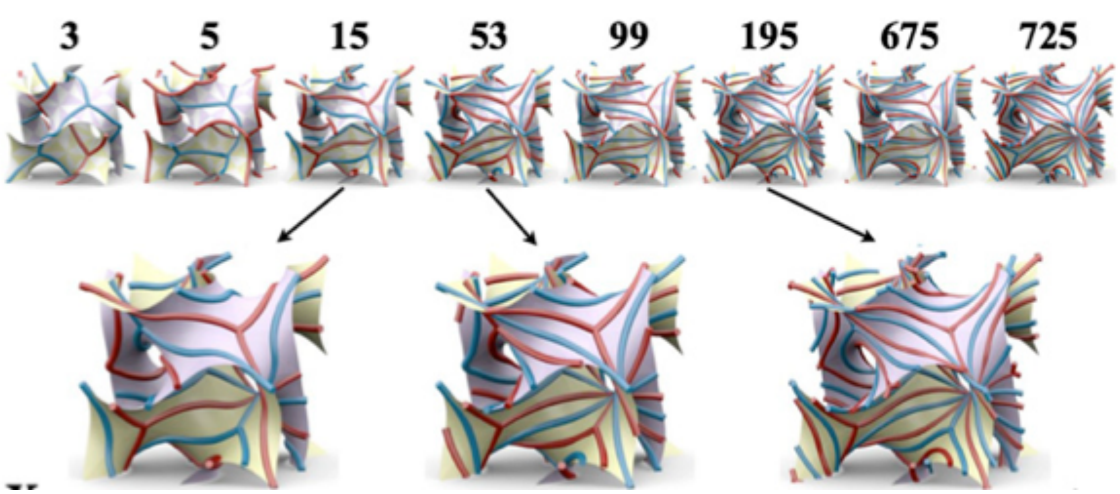


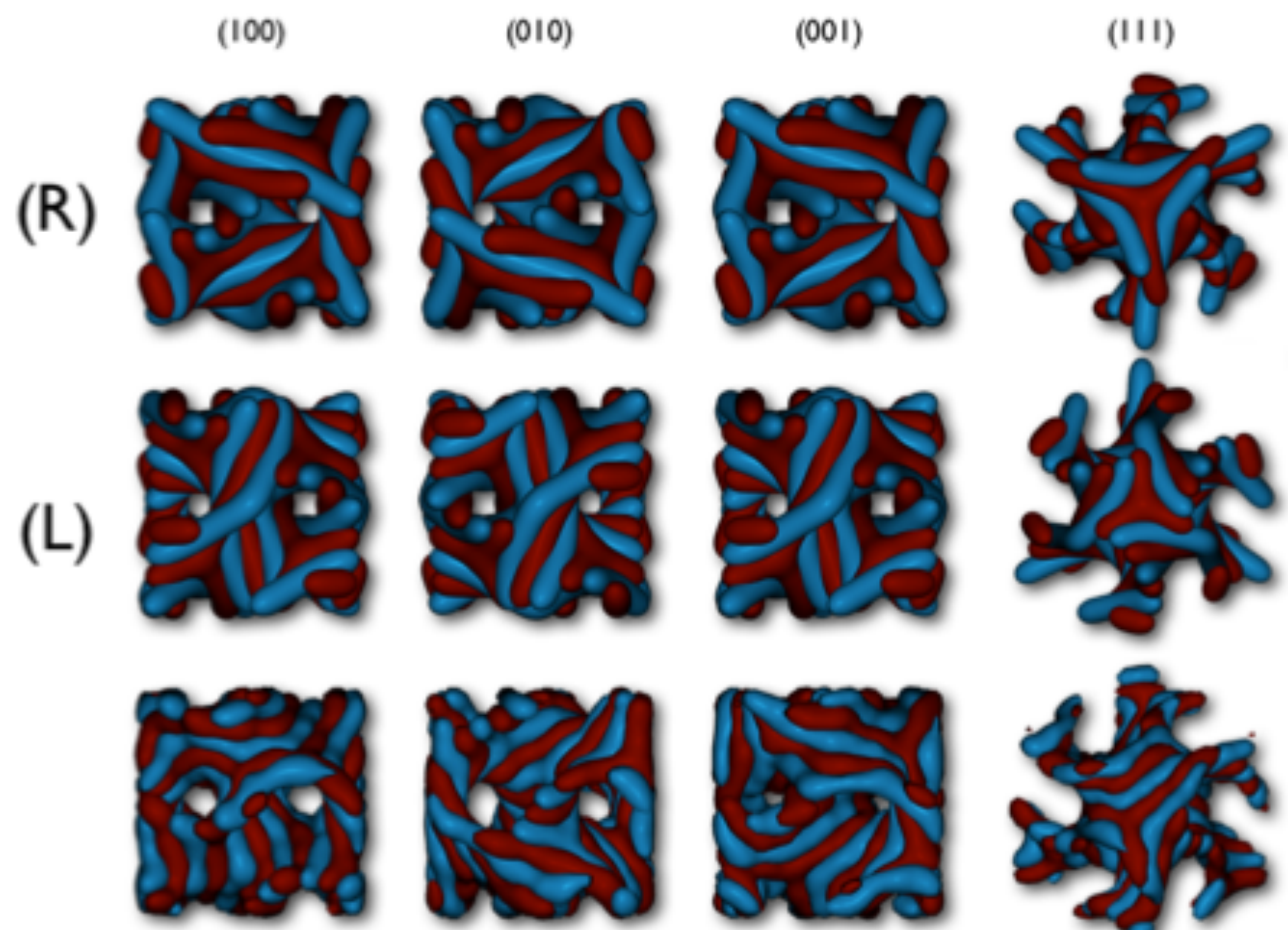


Ideally, all nets are of the same hand...

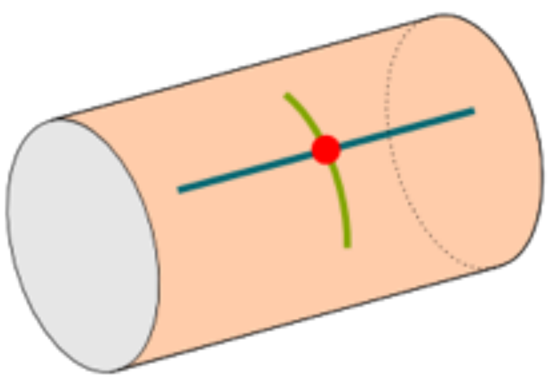




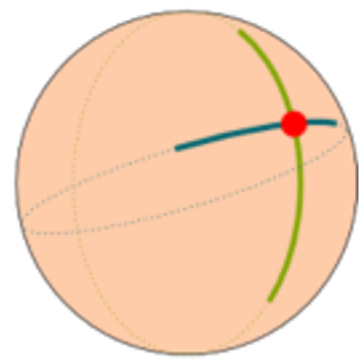




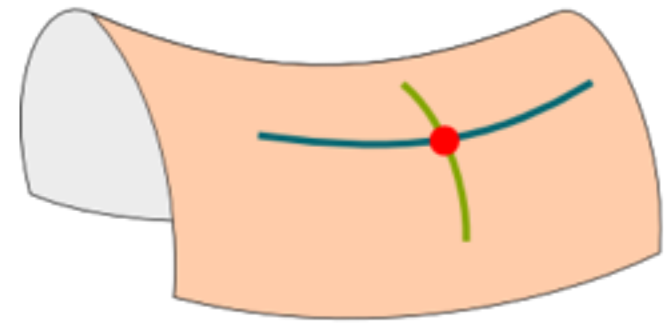
Stars in curved geometries



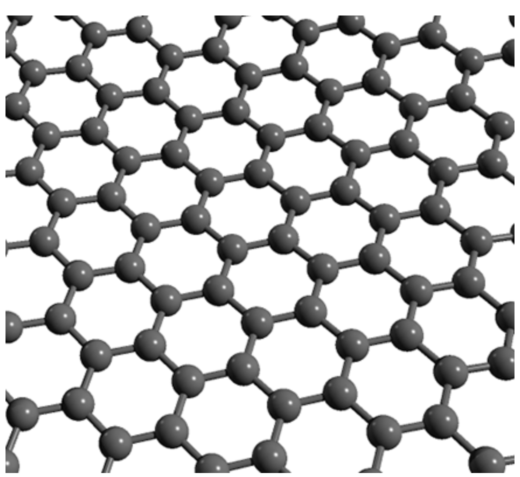
Zero Curvature

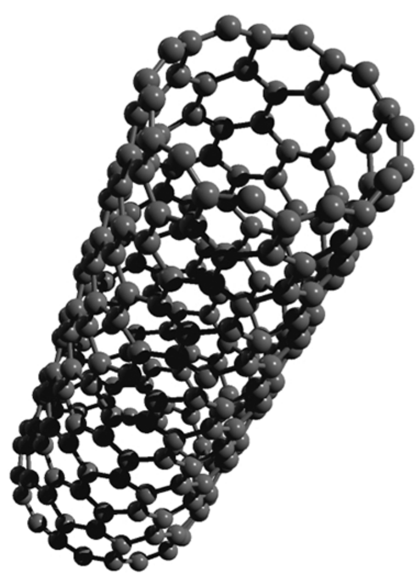


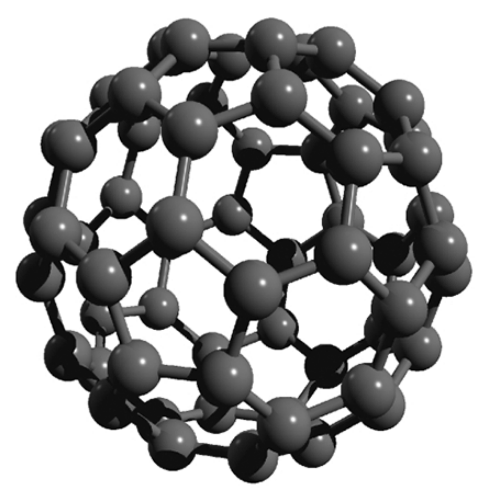
Positive Curvature

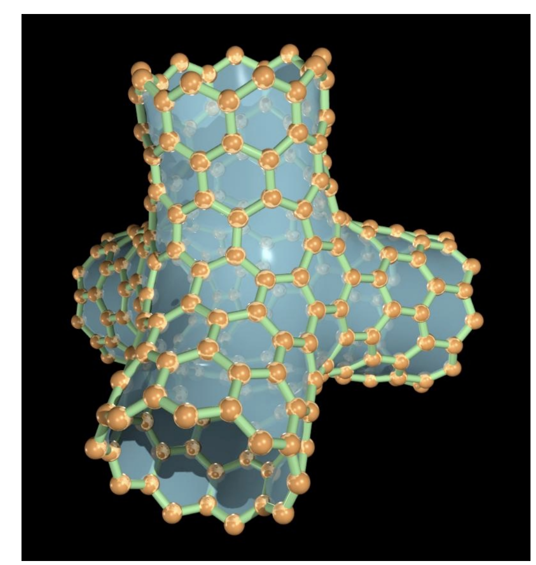


Negative Curvature





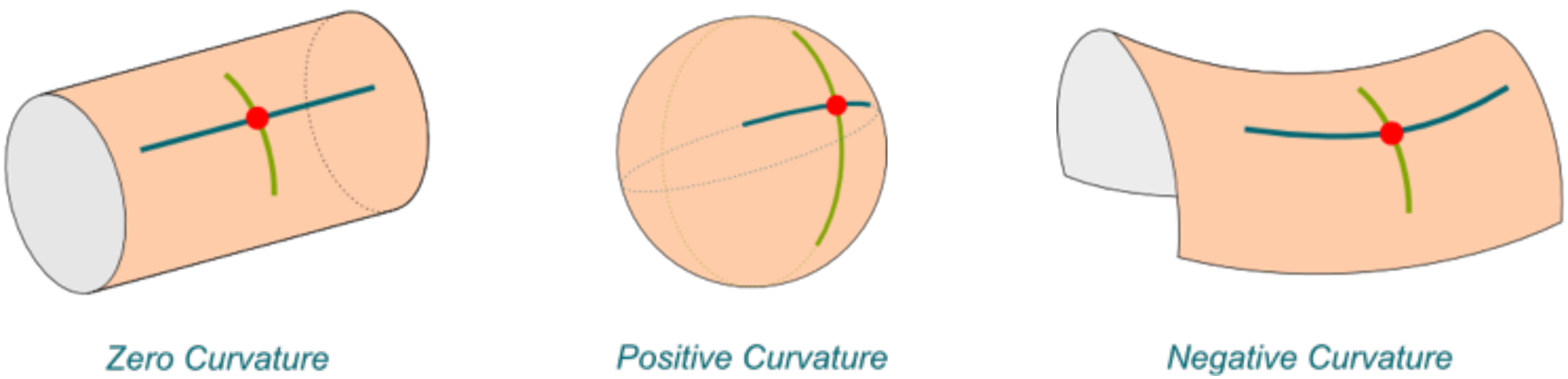


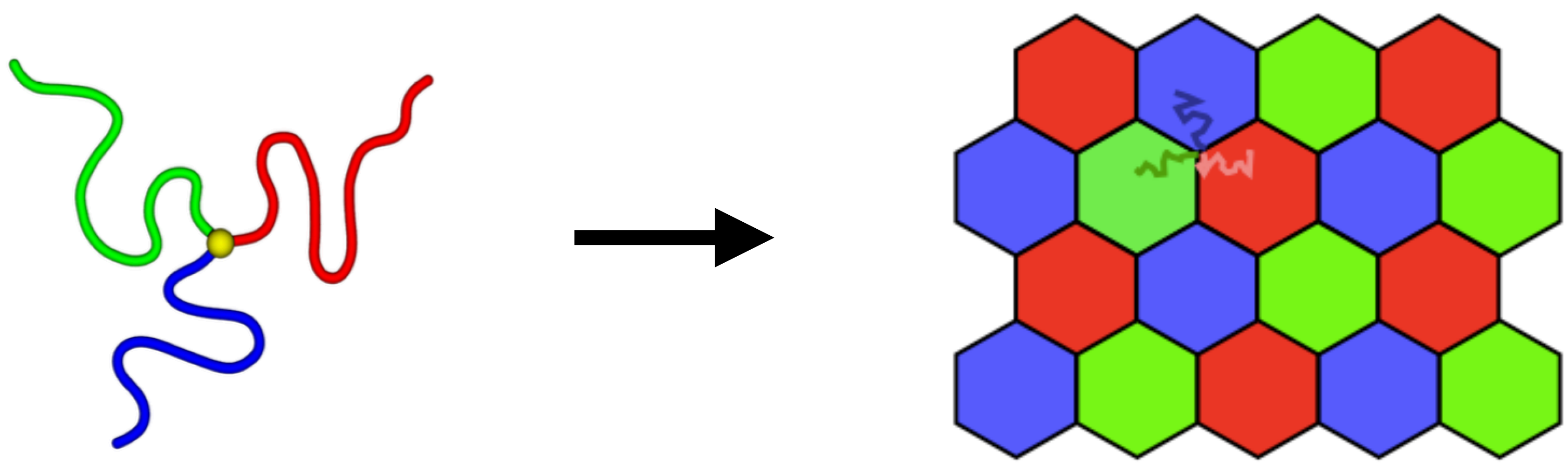


Images: Jan Smotlacha

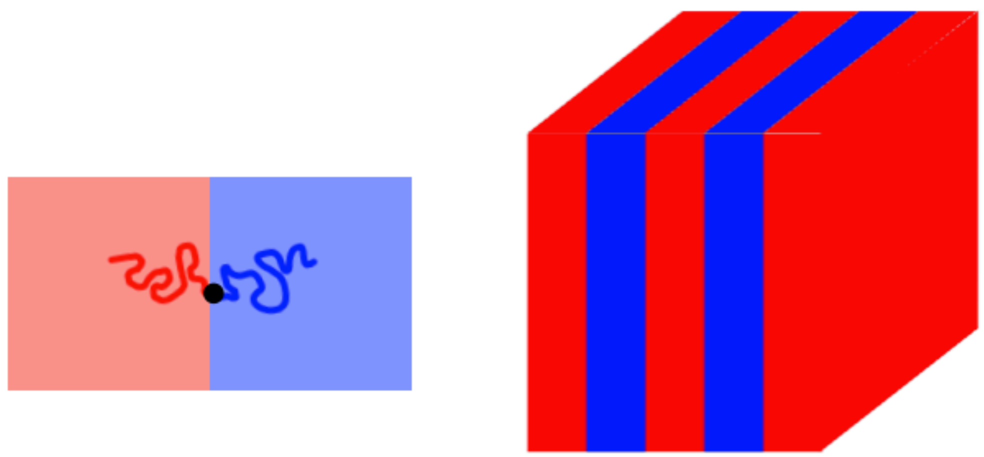
Image: Stu Ramsden, ANU

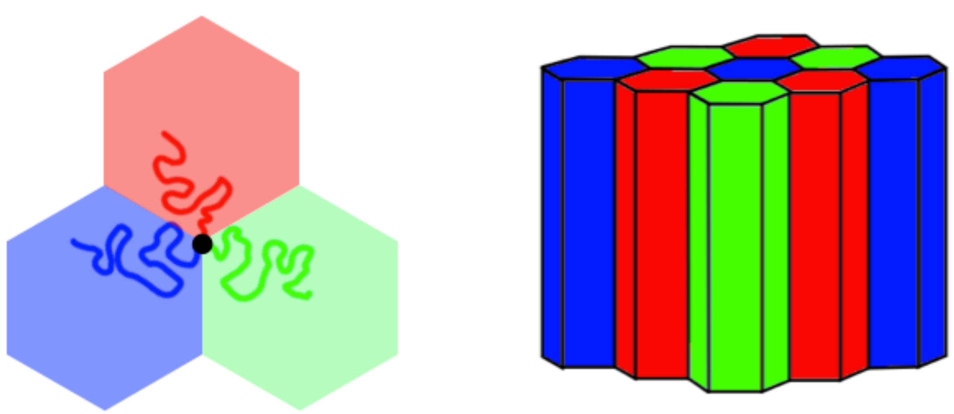
Stars in curved geometries

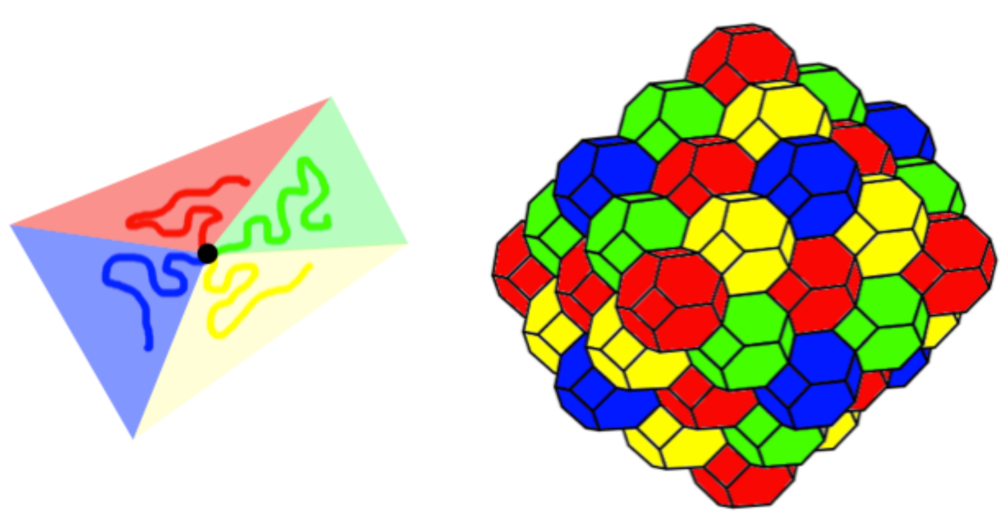




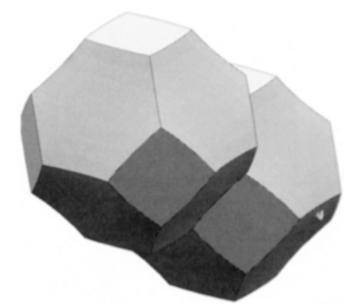
ABCD 4-miktoarm stars



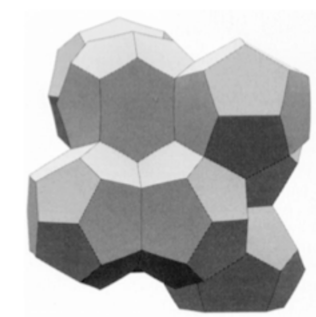




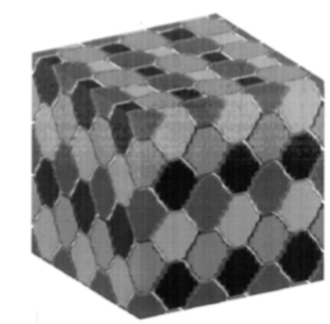
Balanced



Kelvin



Weaire-Phelan

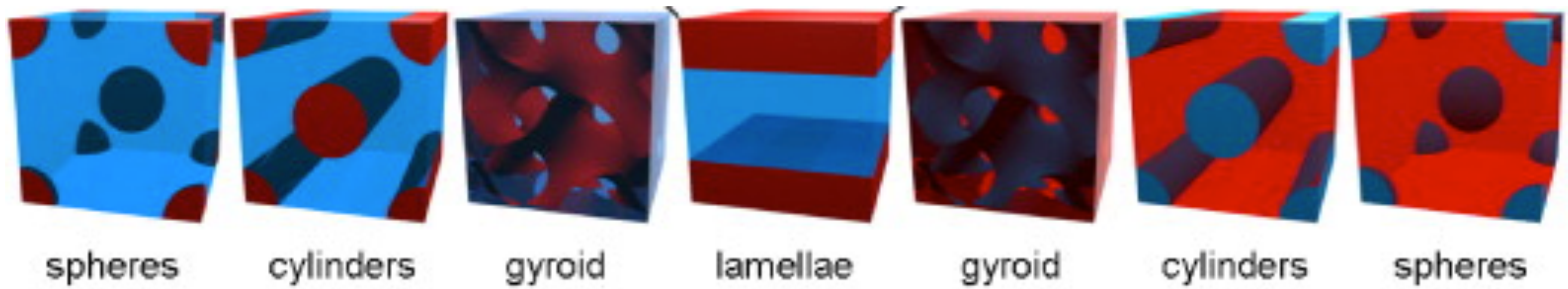


4-colored
Kelvin Foam

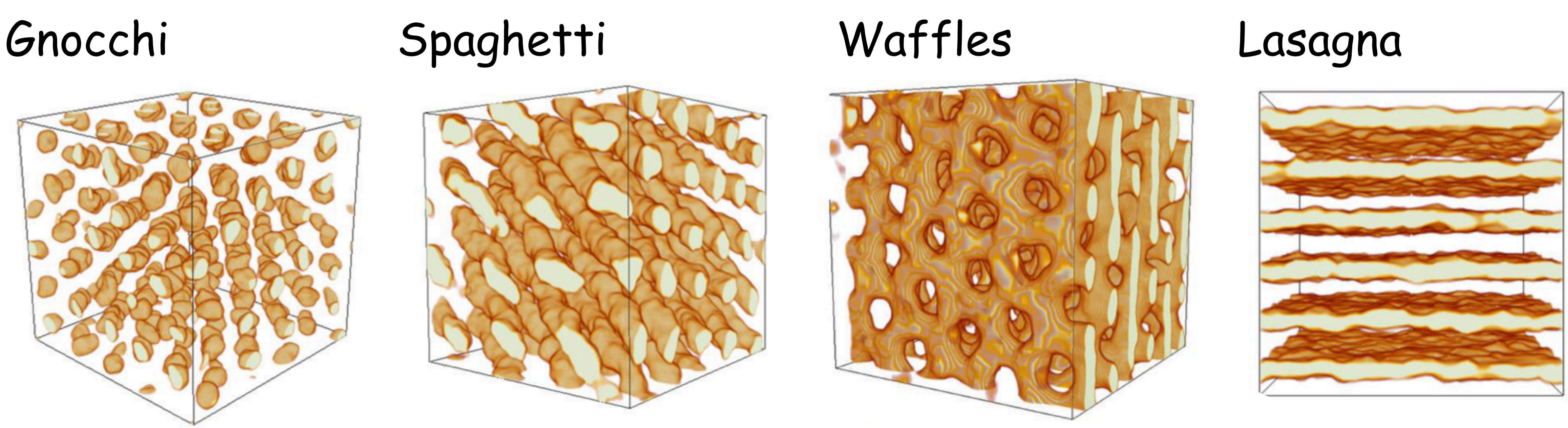
Monte Carlo simulations of ABCD star
Dotera, *Phys. Rev. Let.*, **82**, 1, 1999

The colouring constraint kills the WP foam
(and entropy does also, probably)

BCP self-assembly - relevance to other phenomena



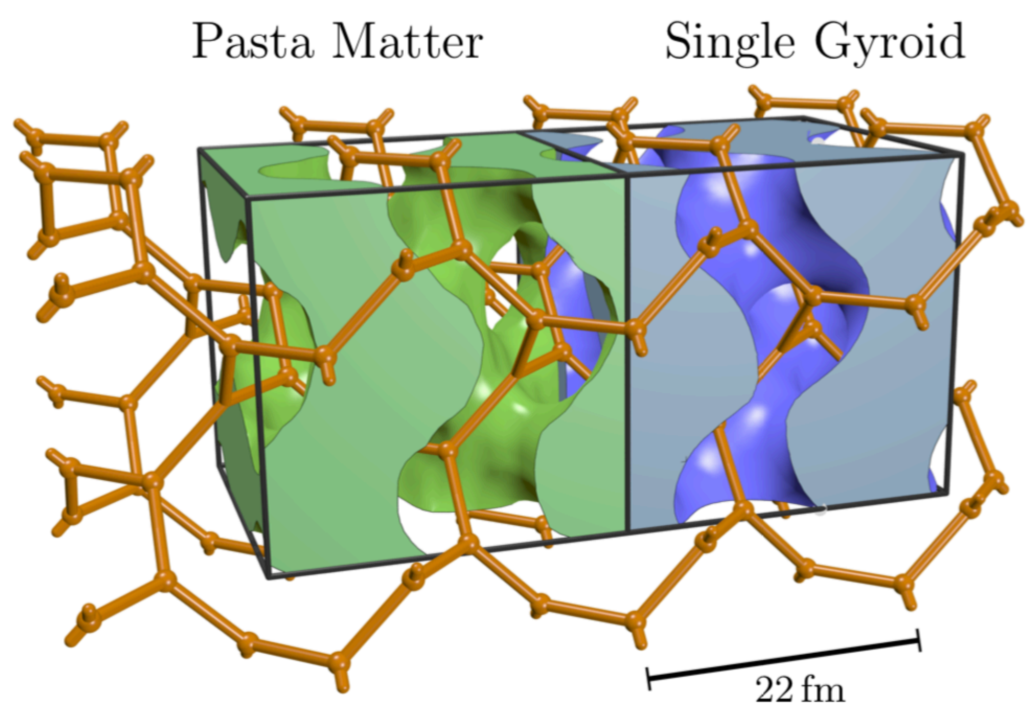
Nuclear pasta (proton density) configurations in inner crusts of neutron stars (at densities of 10^{14} g/cm^3)



Caplan and Horowitz, Rev. Mod. Phys 89, 2017

BCP self-assembly - relevance to other phenomena

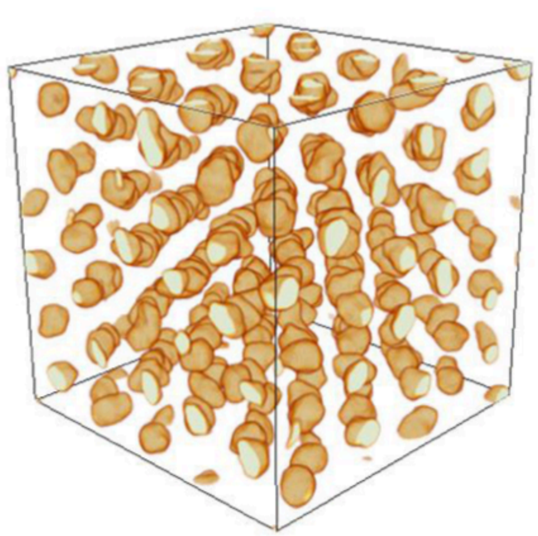
Liquid (high density) phase is filled, gas (low density) phase is void



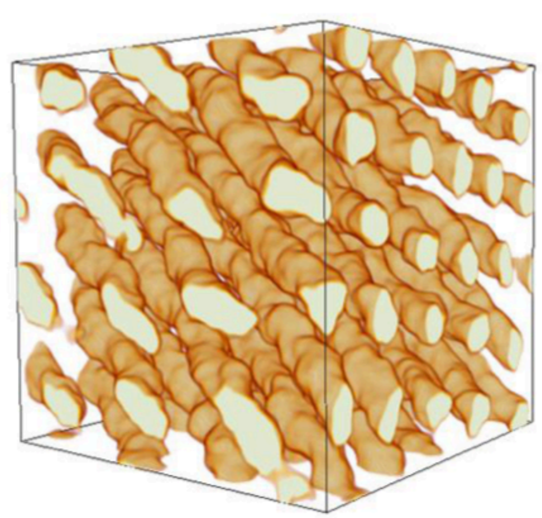
Schuetrumpf et al. Physical Review C 91, 025801 (2015)

Nuclear pasta (proton density) configurations in inner crusts of neutron stars (at densities of 10^{14} g/cm^3)

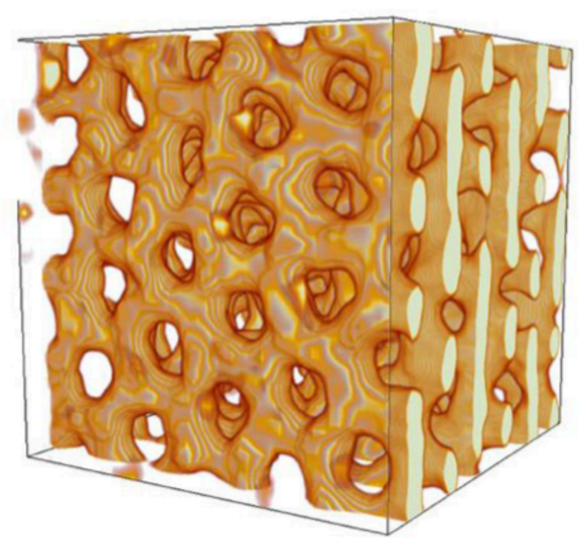
Gnocchi



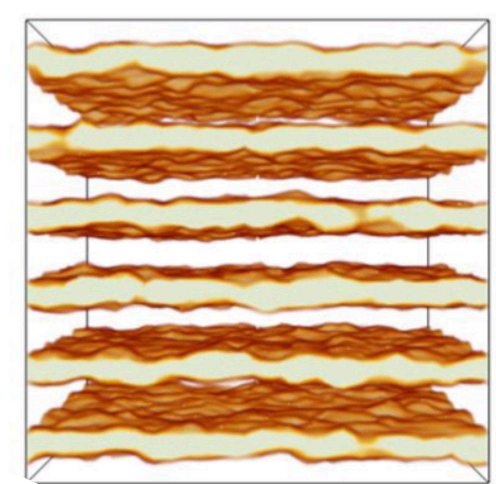
Spaghetti



Waffles

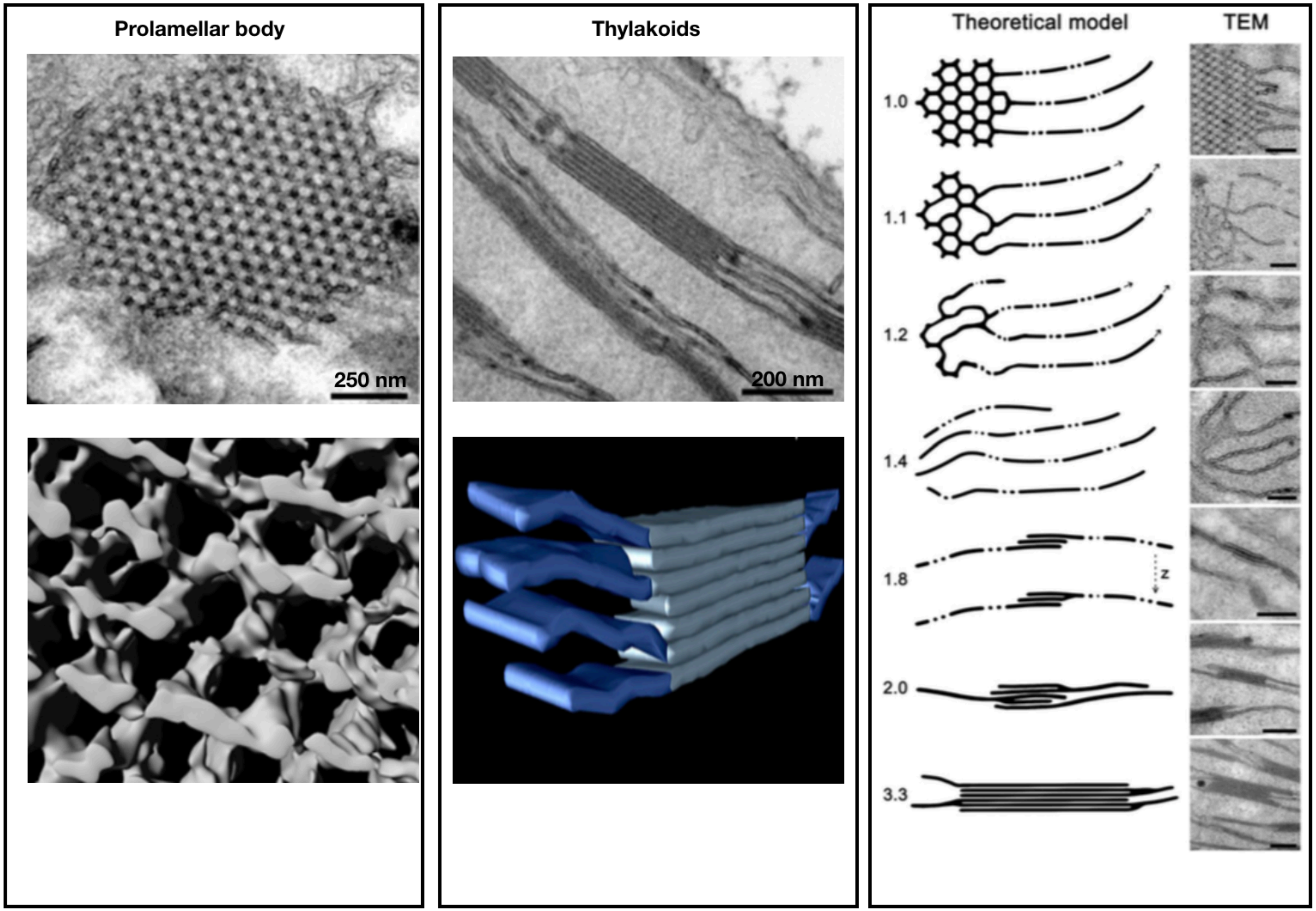


Lasagna



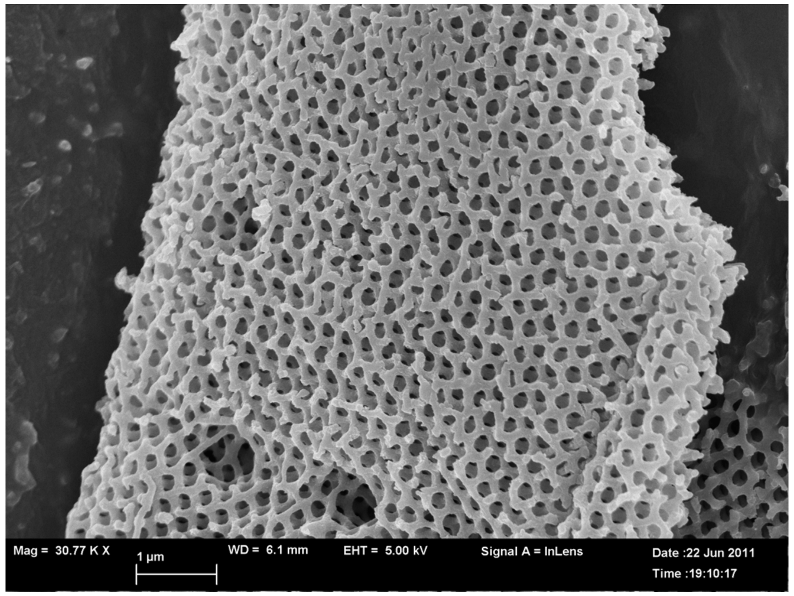
Caplan and Horowitz, Rev. Mod. Phys 89, 2017

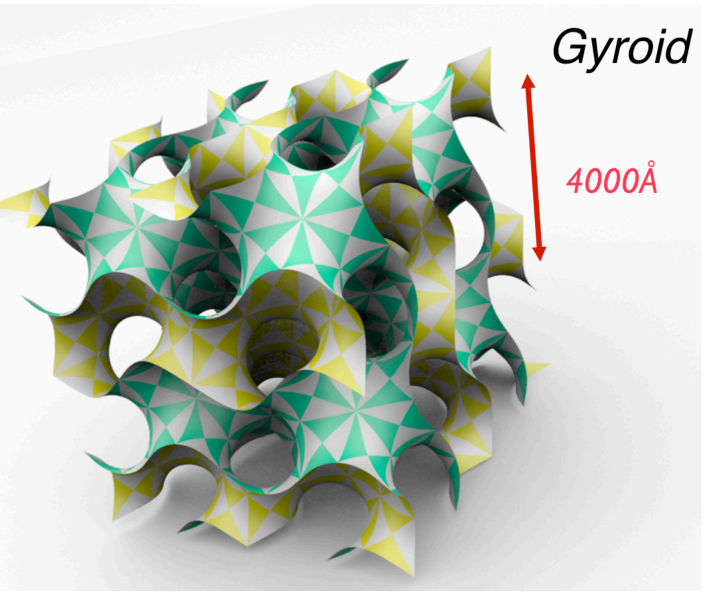
Biology: Cubic-lamellar transition in plant membranes

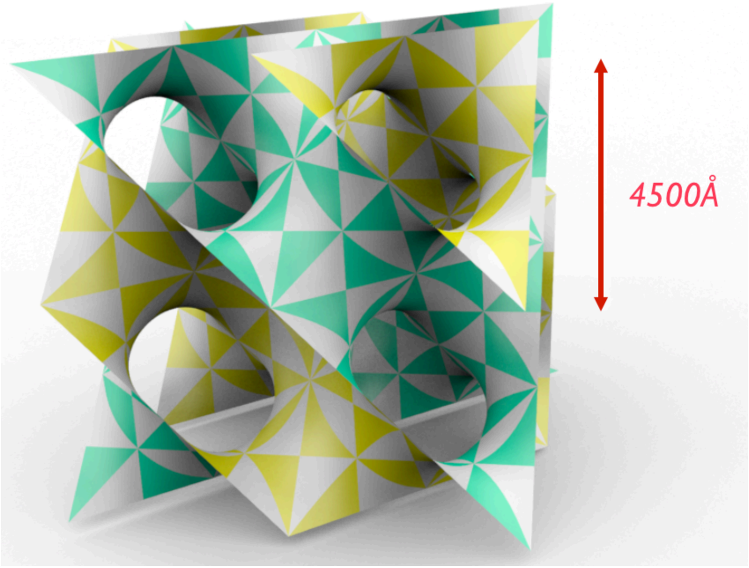


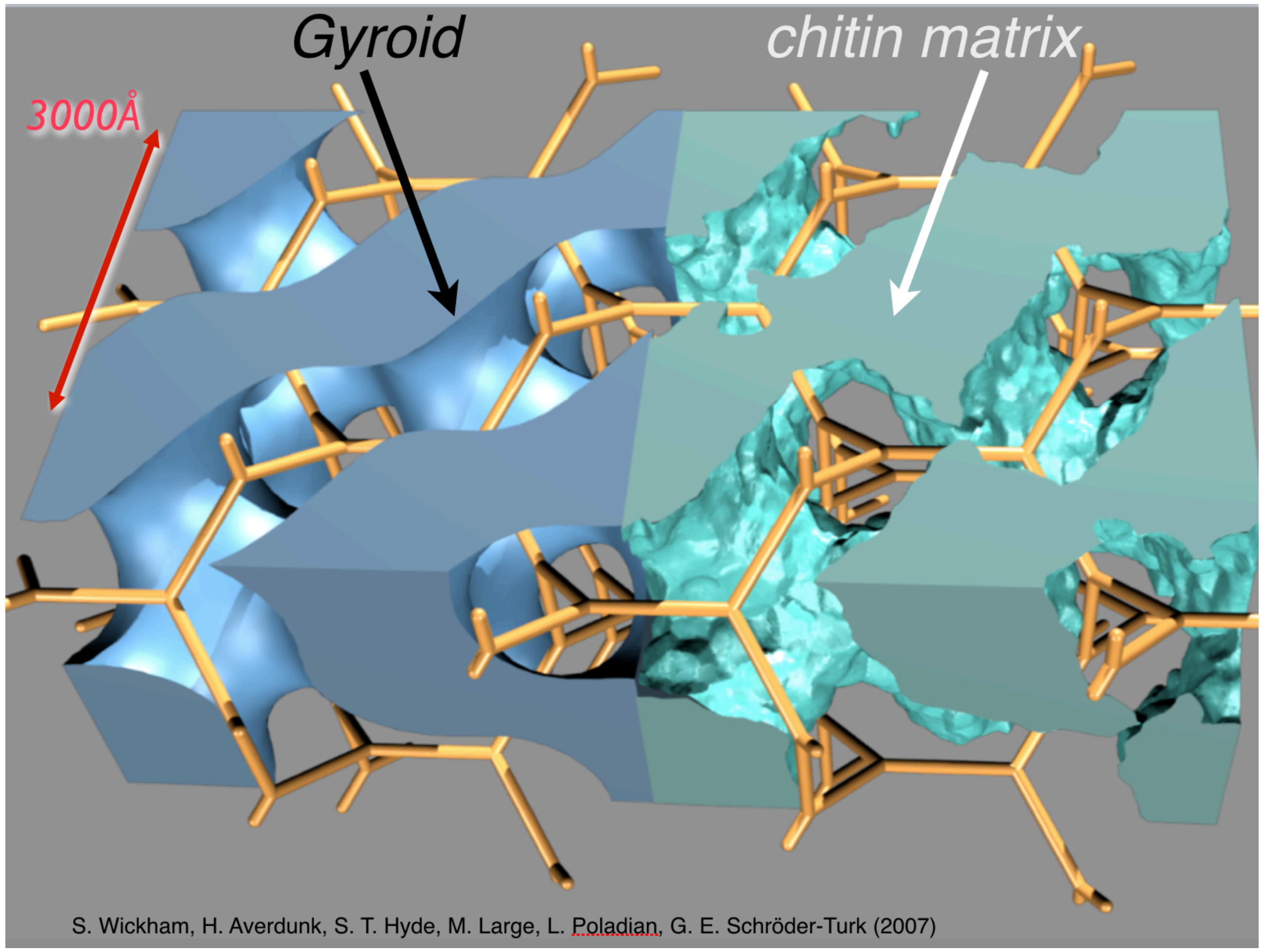
Images courtesy Łucja Kowalewska, University of Warsaw

Biology: Butterflies and weevils









Diamond weevil contains hyperbolic diamond form

Butterfly wings contains hyperbolic gyroid form

Images courtesy Gerd Schröder-Turk, Murdoch University