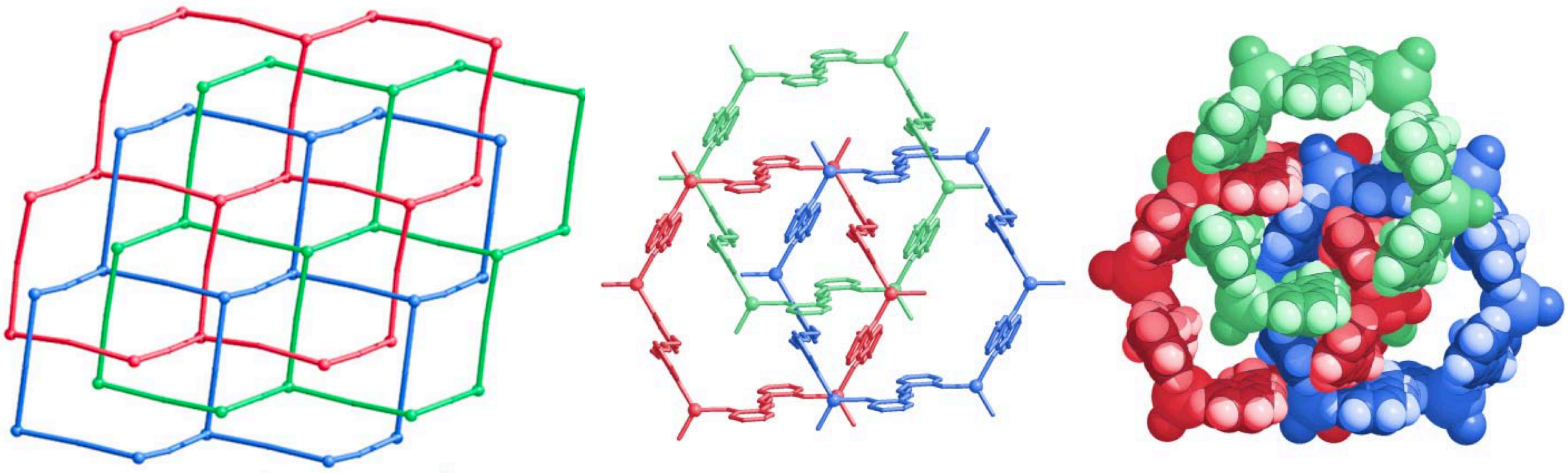
Entanglements of graphs and networks

1: Entanglements in (molecular) networks



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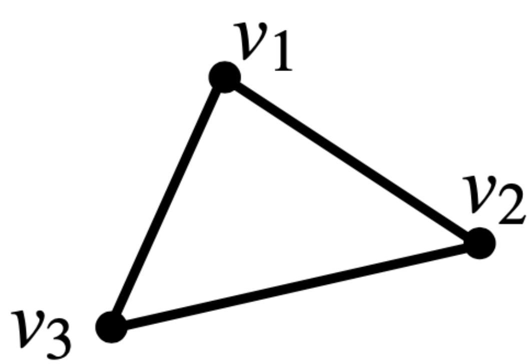
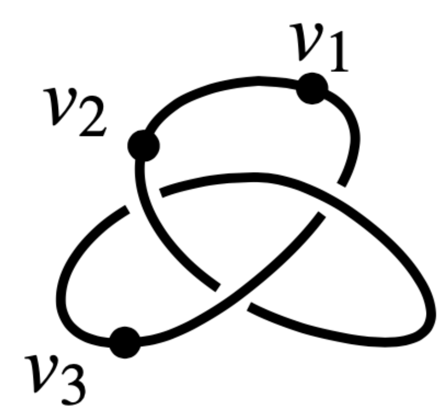
VU UNIVERSITY AMSTERDAM

Entanglements of graphs and networks

Graph: A graph G is a set of vertices together with edges between those vertices.

Spatial graph: A spatial graph $\mathcal{G}$ is the image of an embedding of a graph G into 3-space up to ambient isotopy.





$$\mathcal{G}_1 = g_1(G) \subset \mathbb{R}^2 \qquad \mathcal{G}_2 = g_2(G) \not\subset \mathbb{R}^2 \subset \mathbb{R}^3$$

$$G = \{v_1, v_2, v_3, v_1v_2, v_1v_3, v_2v_3\}$$

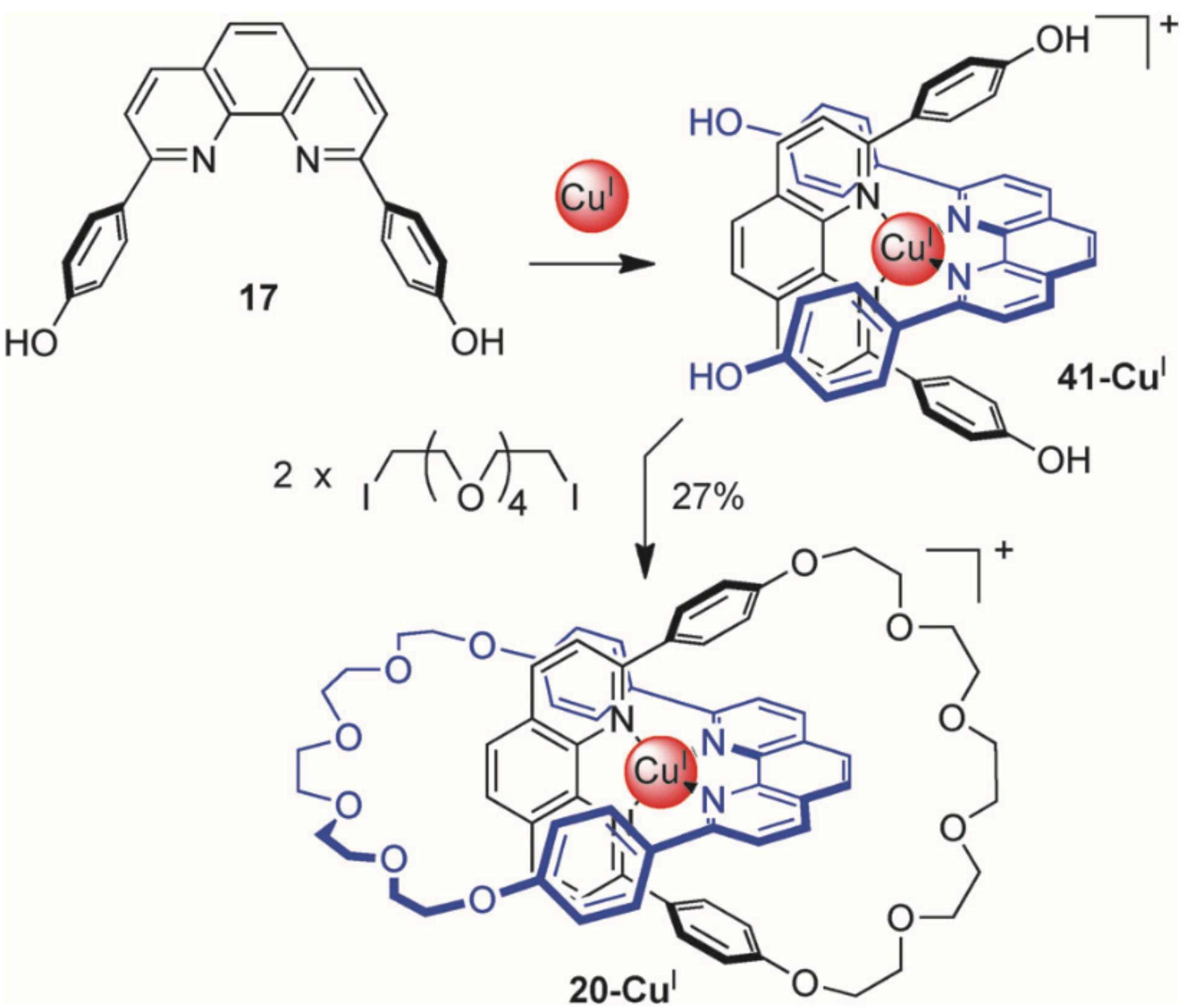
Network (as used in crystallography):

The underlying graph of a crystal (usually extended in 3, at least 2 directions).
A periodic graph extending in two or three undefended directions.

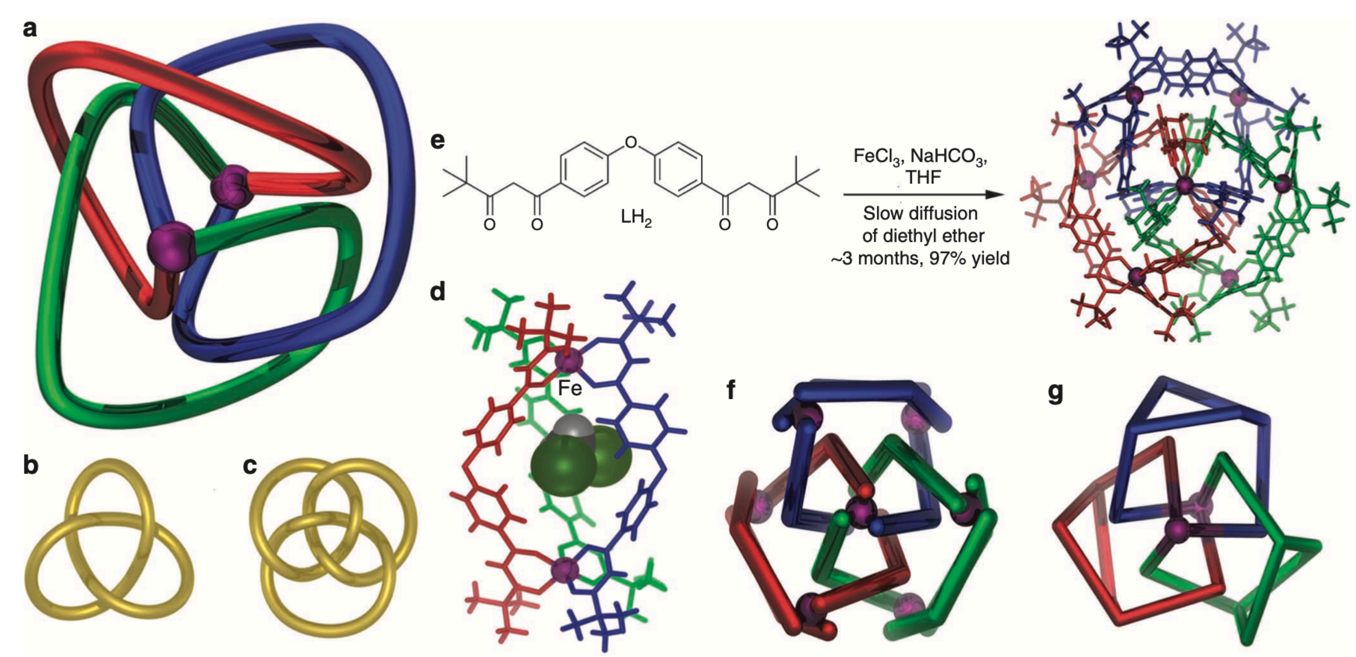
Entanglements of graphs and networks

Entanglement of spatial graphs: - knot theory (knots)
- topological graph theory (different notions, see later) (depends on the graph **and** on the embedding)

Entanglements in molecules : - single molecules (synthetic: 3_1,4_1,5_1,7_4,8_1,8_{19}, links)



Christiane O. Dietrich-Buchecker, Jean-Pierre Sauvage: 1989



Feng Li, Jack K. Clegg, Leonard F. Lindoy, René B. Macquart, George V. Meehan: 2011

Entanglements of graphs and networks

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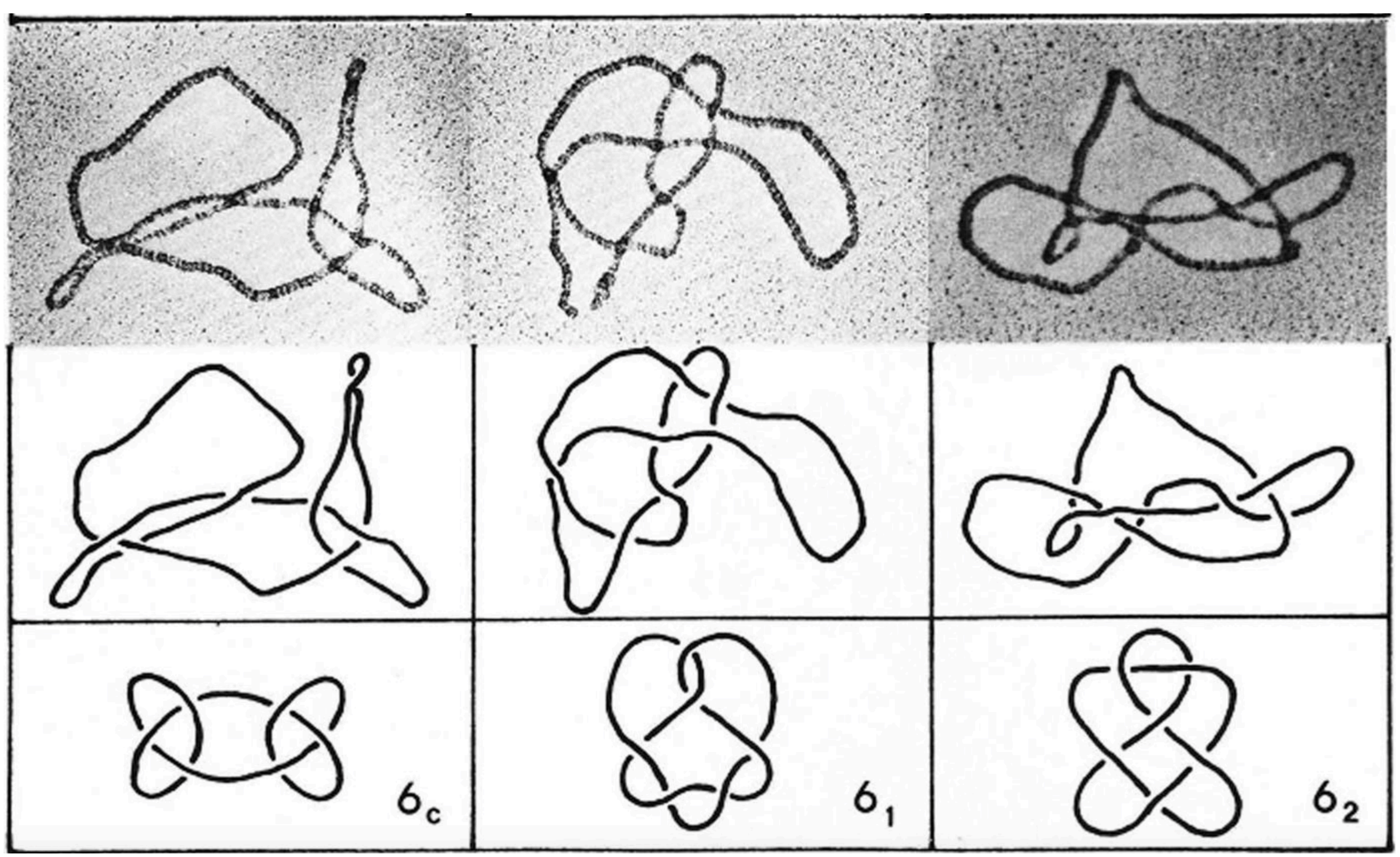
Entanglements in molecules :
- single molecules
- DNA (synthetic and natural)



Dean, Stasiak, Koller, Cozzarelli: 1985

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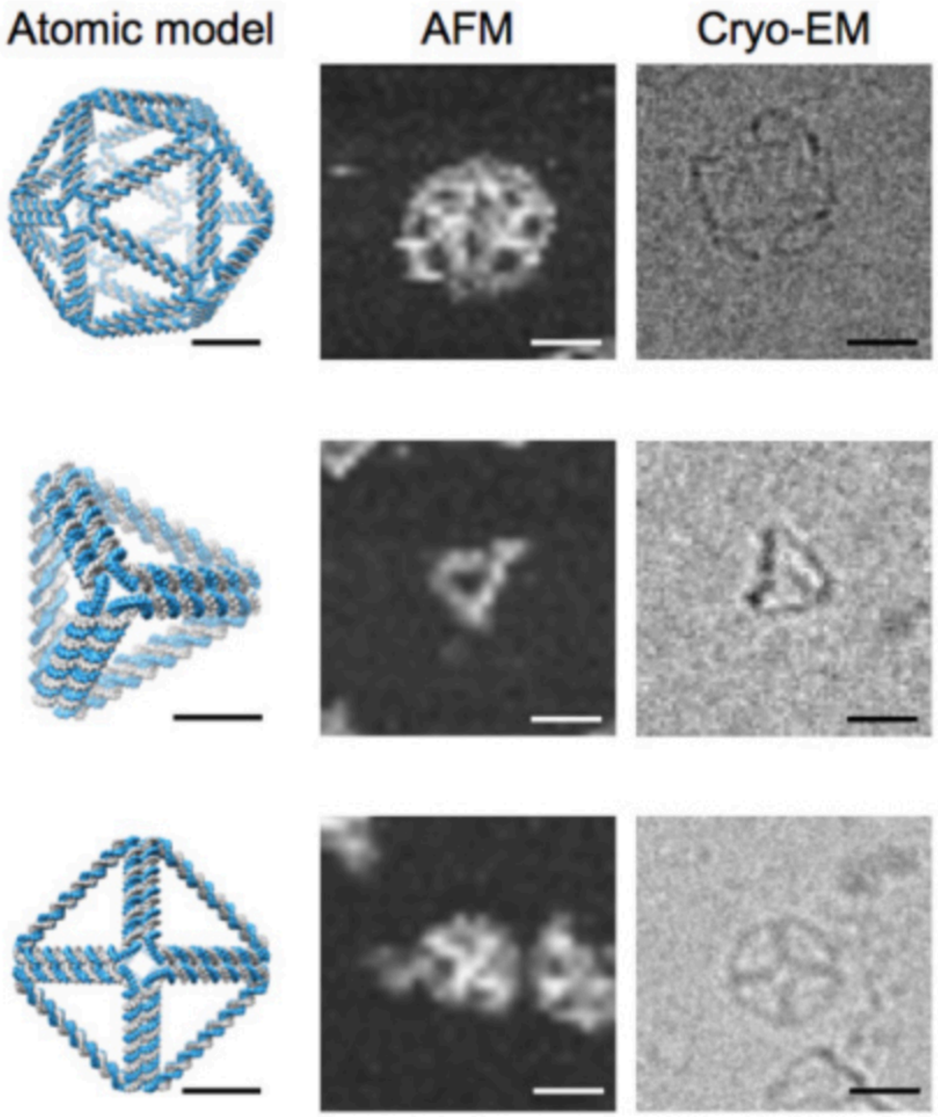

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Entanglements in molecules :
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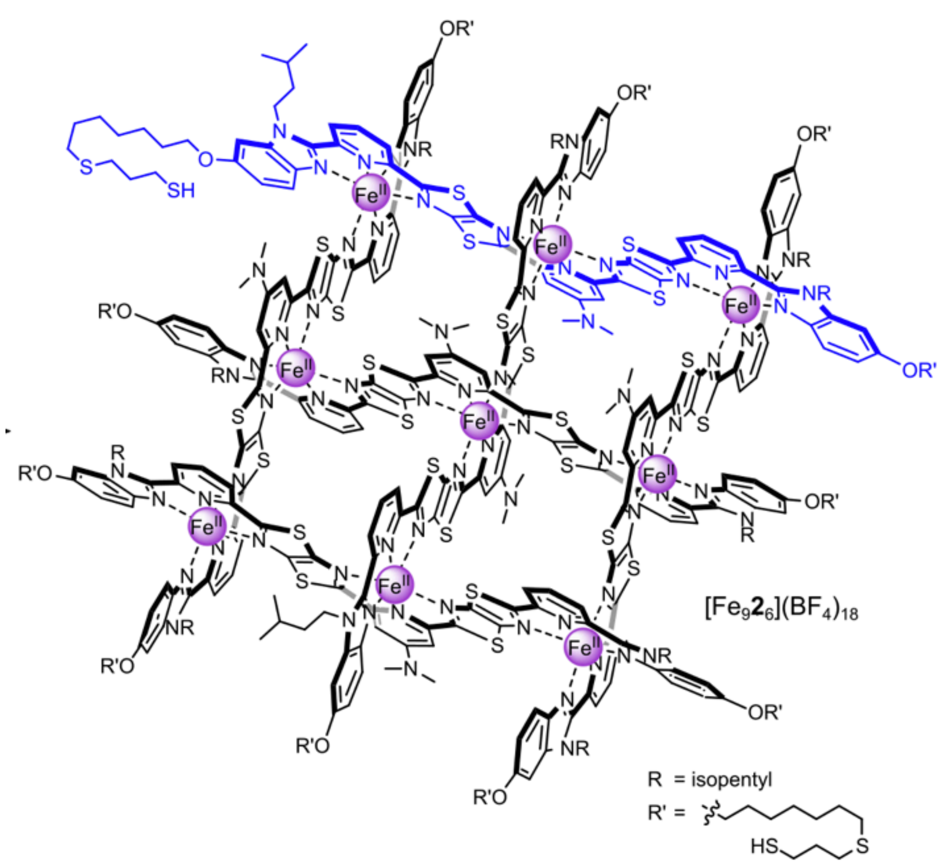
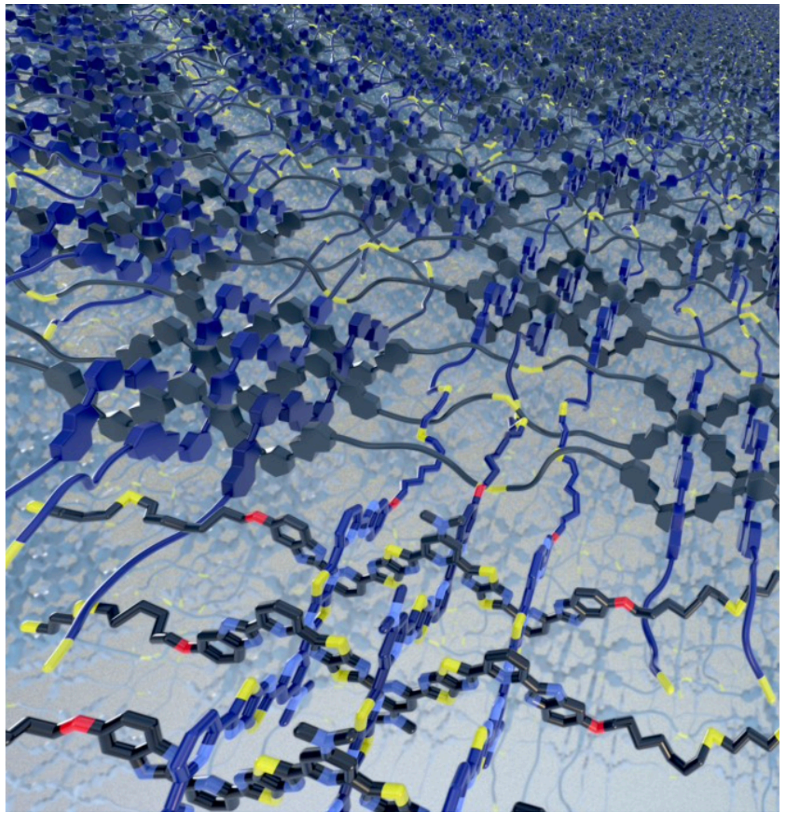
- crystals (designed)





August, Dryfe, Haigh, Kent, Leigh, Lemonnier, Li, Muryn, Palmer, Song, Whitehead, Young: 2020

Entanglements of graphs and networks

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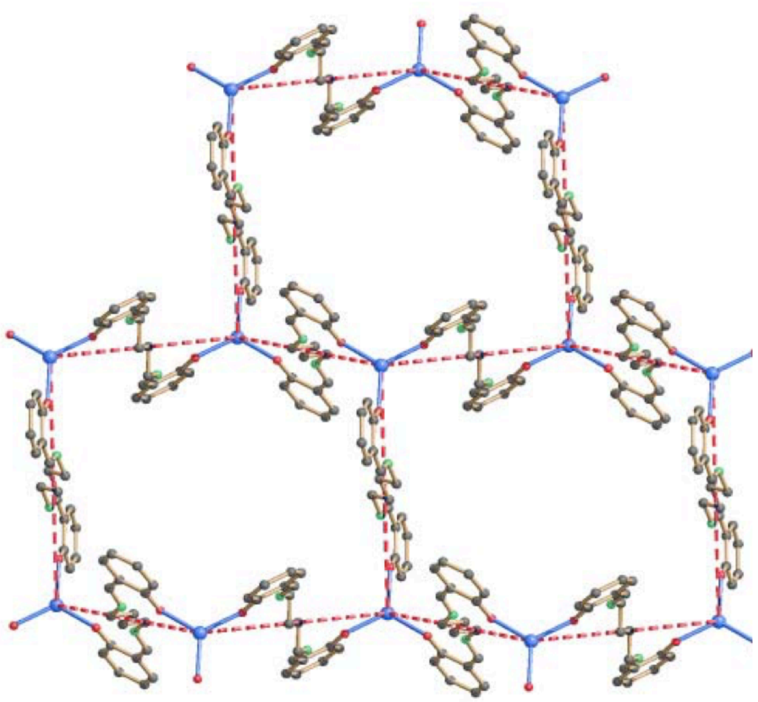
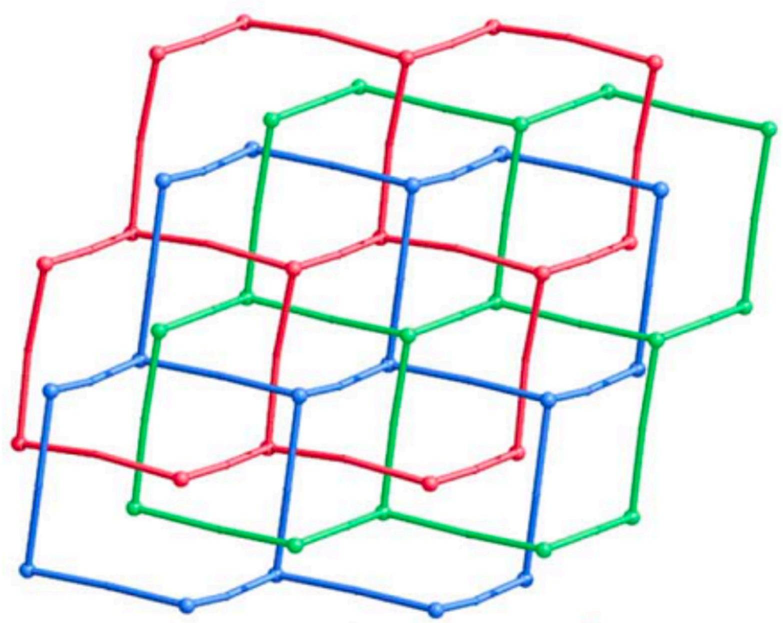
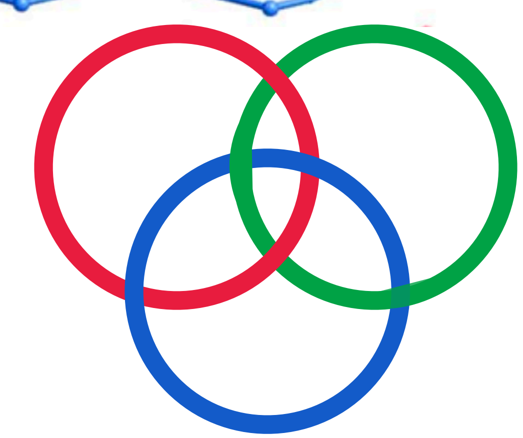
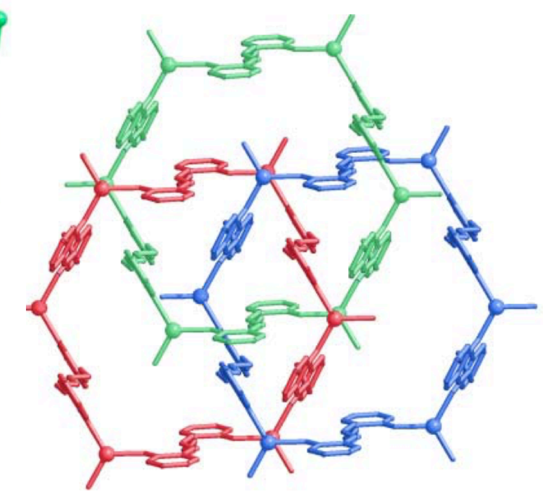
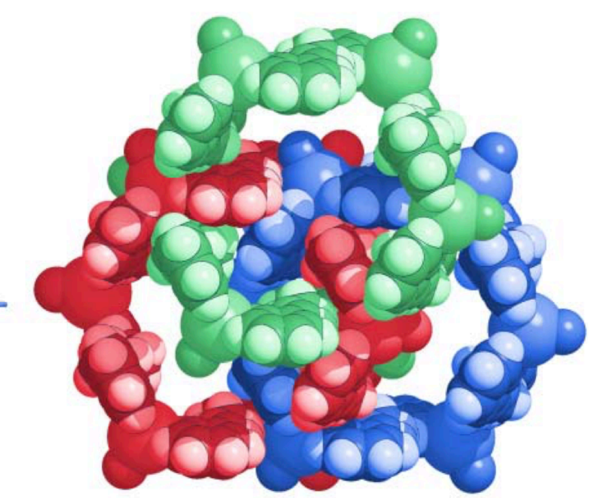
Entanglements in molecules :
- single molecules
- DNA (synthetic and natural)
- crystals (included)







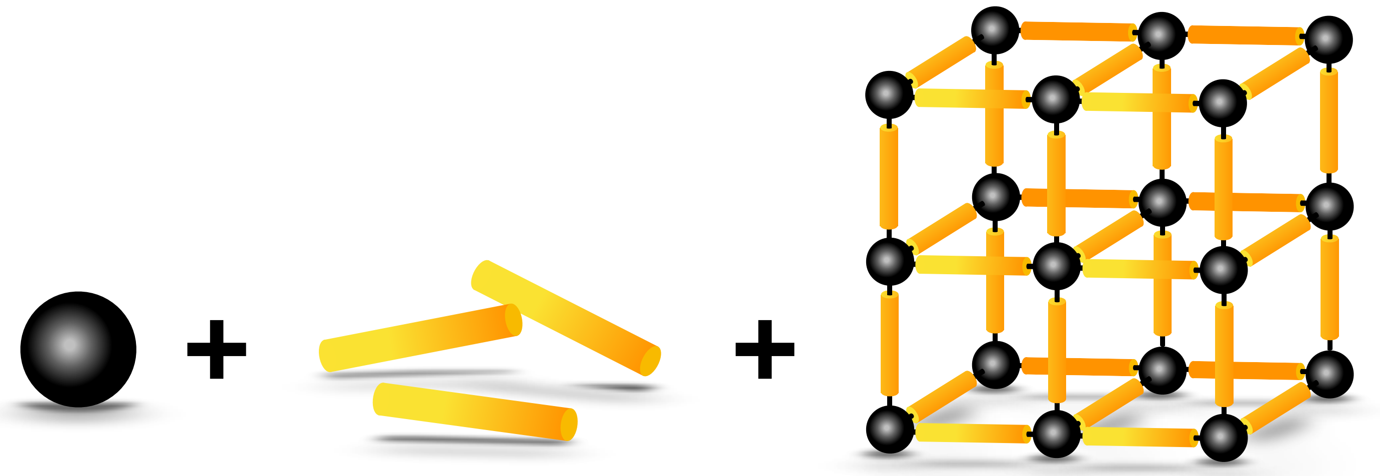


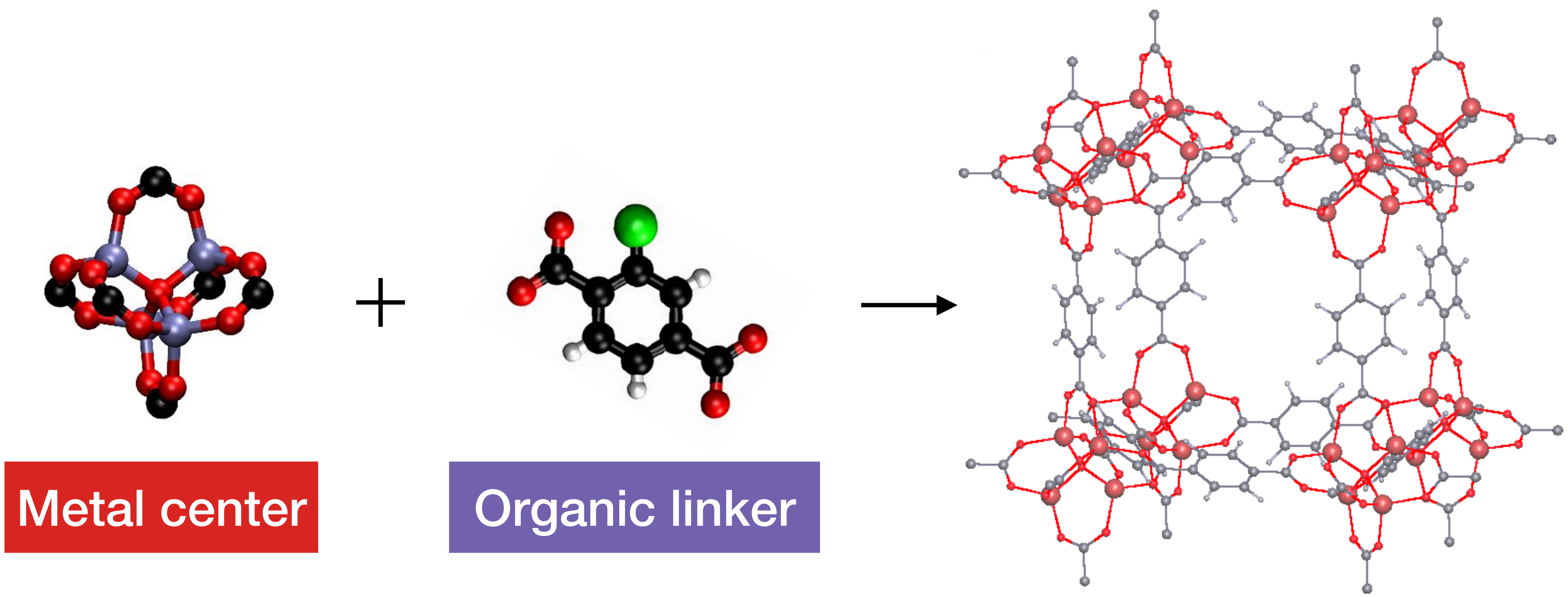


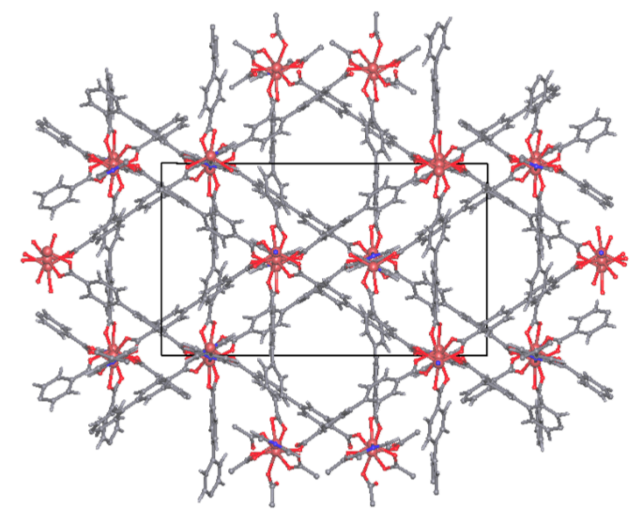
Synthesised by Tong, Chen, Ye, Ji: 1999

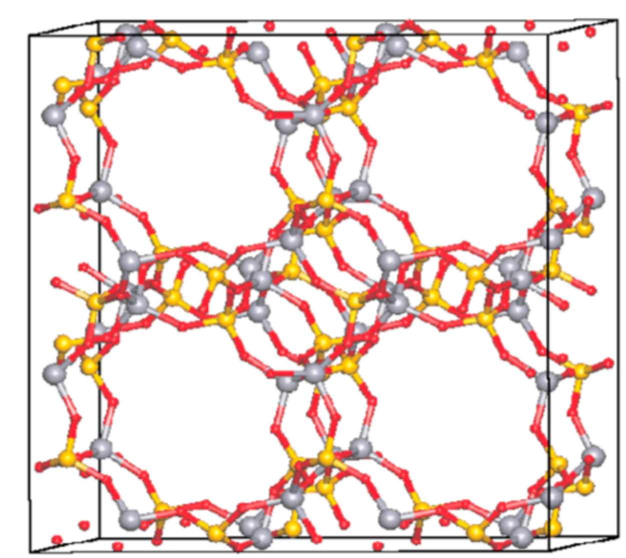
Identified by Carlucci, Ciani, Proserpio: 2003

Entanglements in coordination polymers

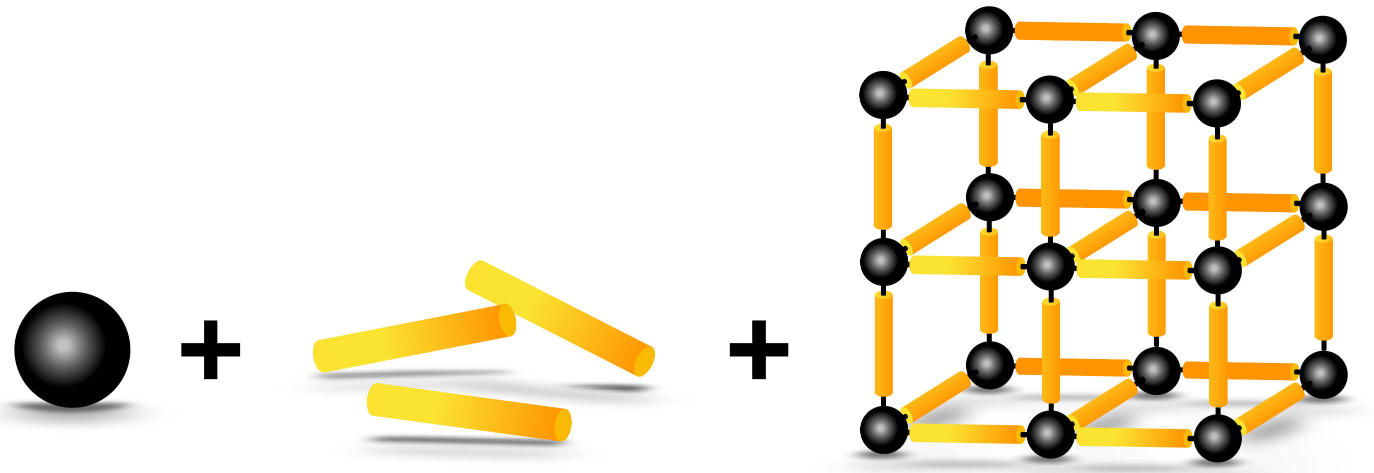


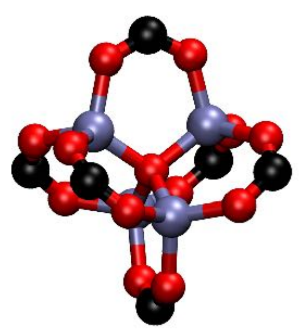




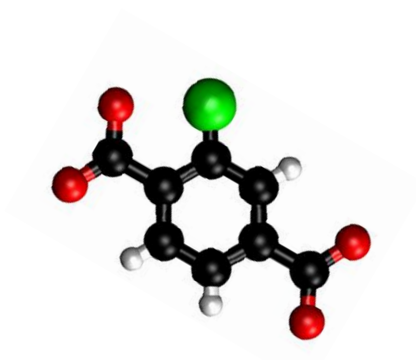


Entanglements in coordination polymers

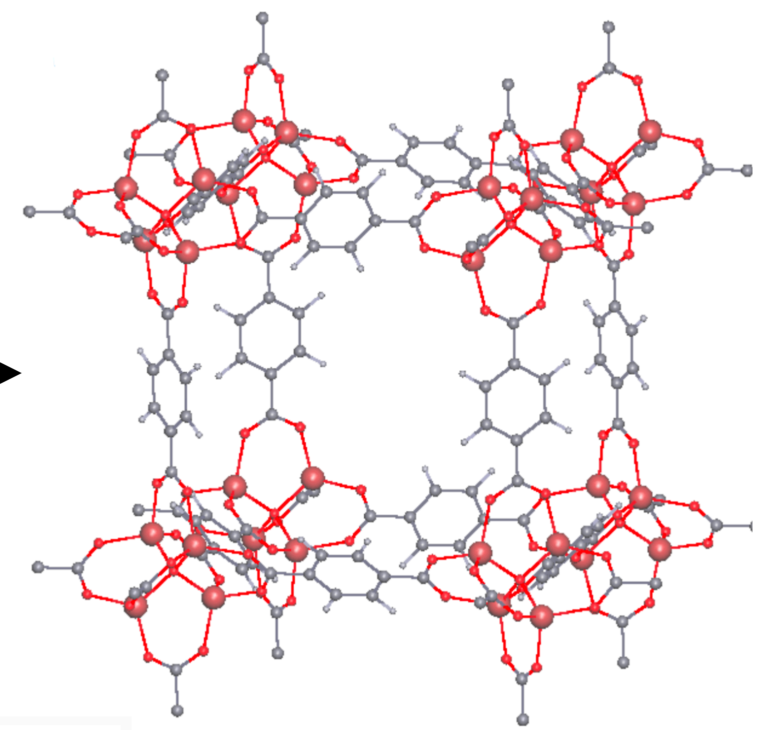


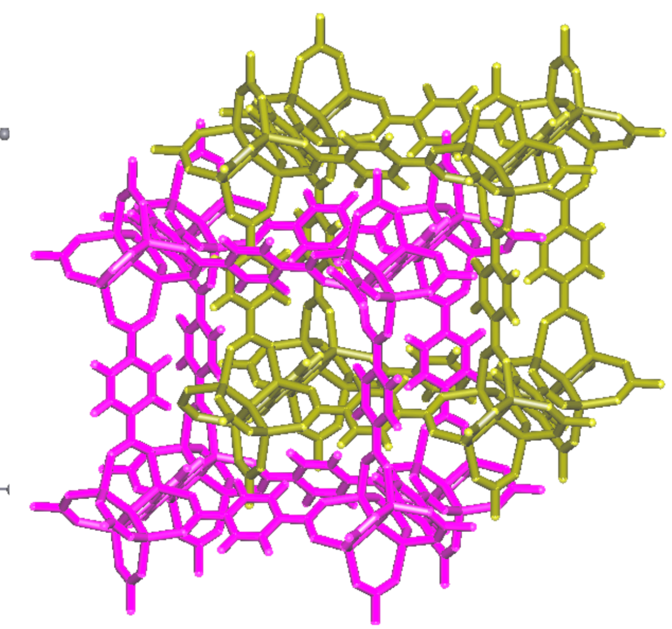


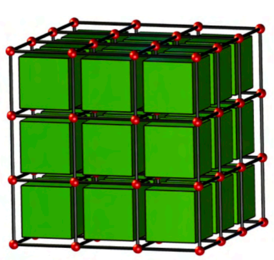
Metal center

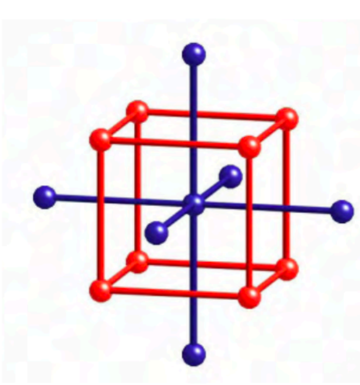


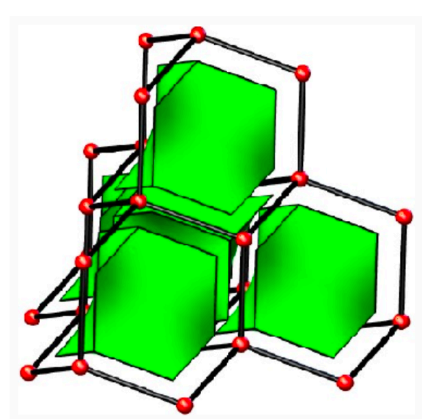
Organic linker

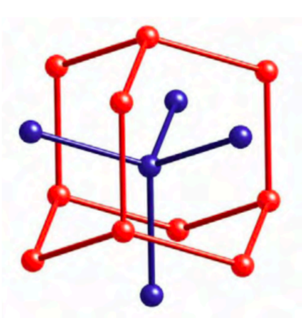




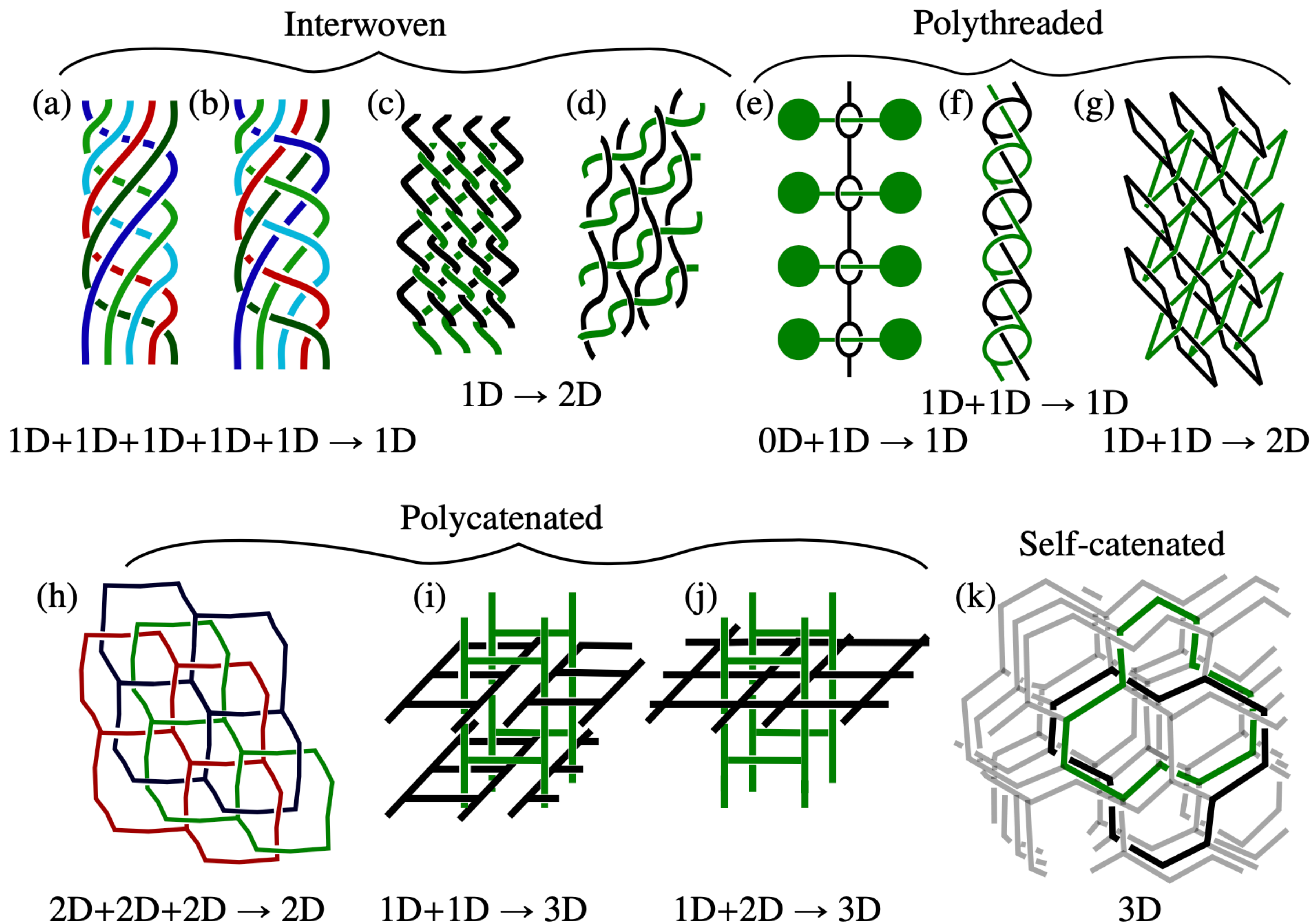








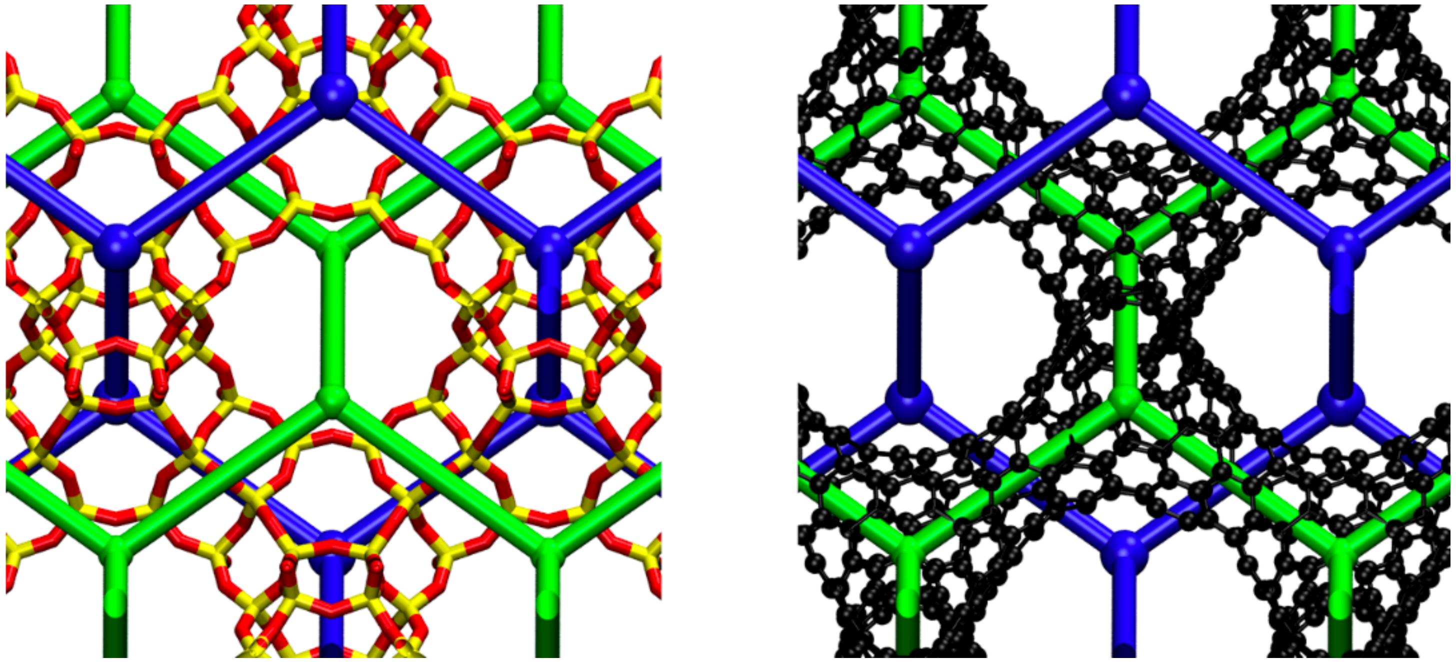
Entanglements in coordination polymers



Entanglements and surfaces

1) Graph embedded on a surface. Complexity measurement of the graph embedding.

2) Interested in surfaces. Usually three periodic (often minimal surfaces) ⟶ hyperbolic.
Just as the nets before, these can be interpenetrated. **(Myf's talk)**



Braun, Lee, Moosavi, Barthel, Mercado, Baburin, Proserpio, Smit: 2018

Entanglements in spatial graphs

Definitions of the unknot: The only knot that

- is embedded in the plane ($\mathbb{S}^2$)
- bounds a properly embedded disc
- has a complement with free fundamental group ($\mathbb{Z}$, free of rank 1)

These notions are equivalent

Definitions of entanglement-free spatial graphs:

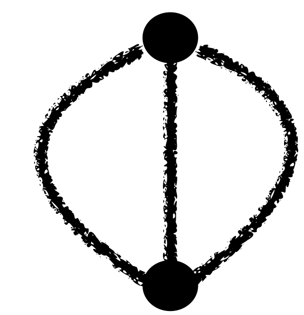
- Knotfree: contains no cycle that is knotted
- Trivial: is embedded in the plane ($\mathbb{S}^2$)
- Panelled: each cycle bounds a properly embedded disc, whose interior is disjoint from the graph
- Free: has a complement with free fundamental group ($\mathbb{Z}^n$, free of rank n)

These notions are not equivalent $\Rightarrow$ many different notions of entanglements

How are these notions related?

Entanglements in spatial graphs

Definitions of entanglement-free spatial graphs:



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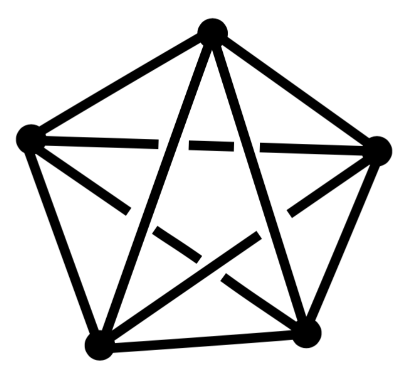
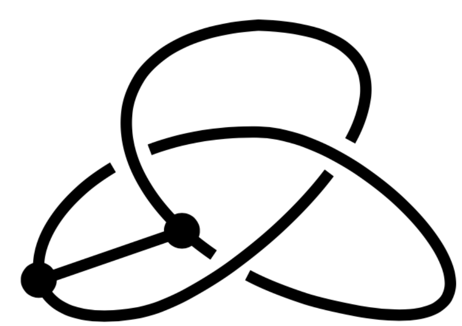
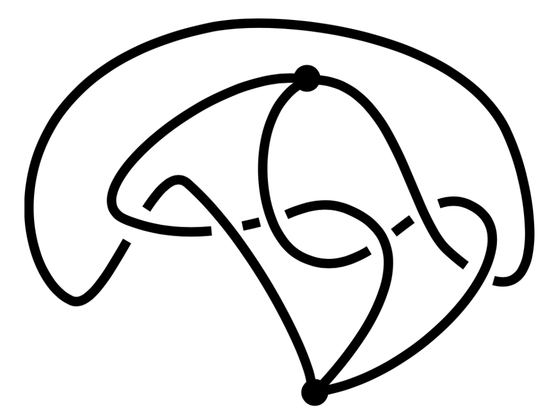
- (Abstractly) planar: the graph admits a trivial embedding

knotfree			
trivial			
(abstractly) planar	✗	✓	✓
panelled			
free			

Entanglements in spatial graphs

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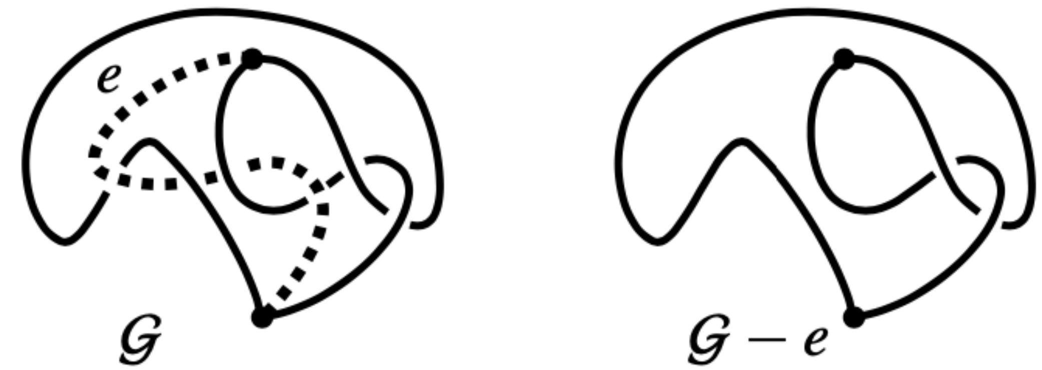

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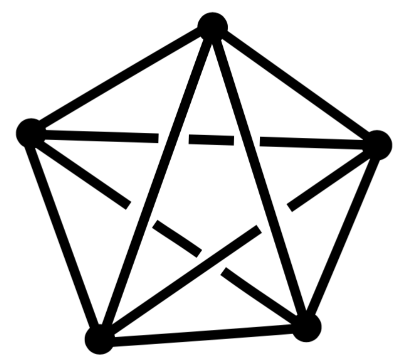

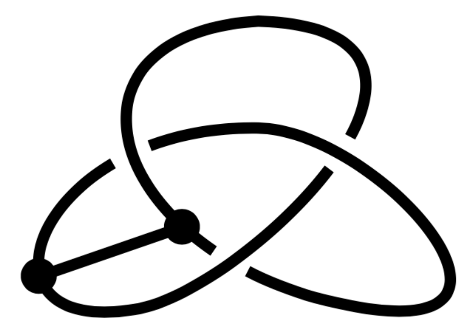

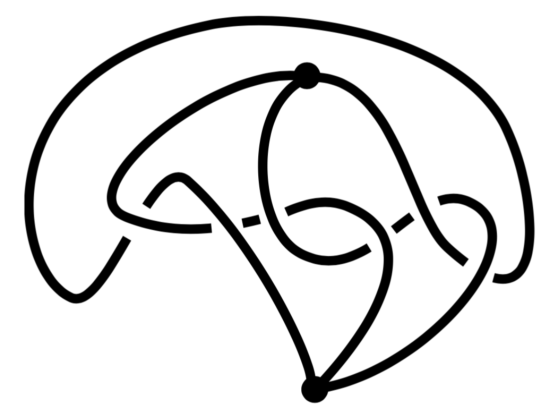

knotfree	✓	✗	✓
trivial			
(abstractly) planar	✗	✓	✓
panelled			
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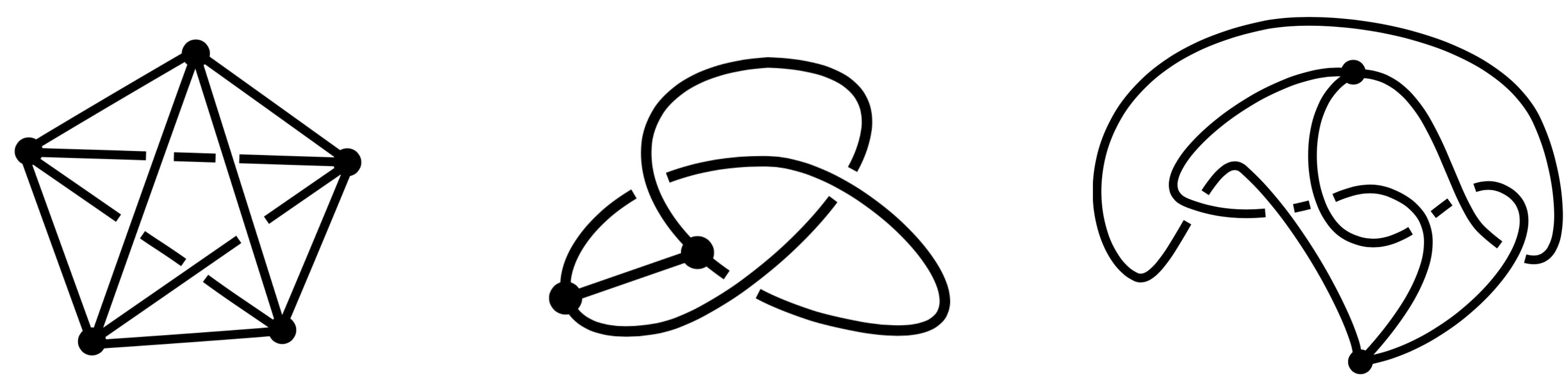

knotfree	✓	✗	✓
trivial	✗	✗	✗
(abstractly) planar	✗	✓	✓
panelled			
free			

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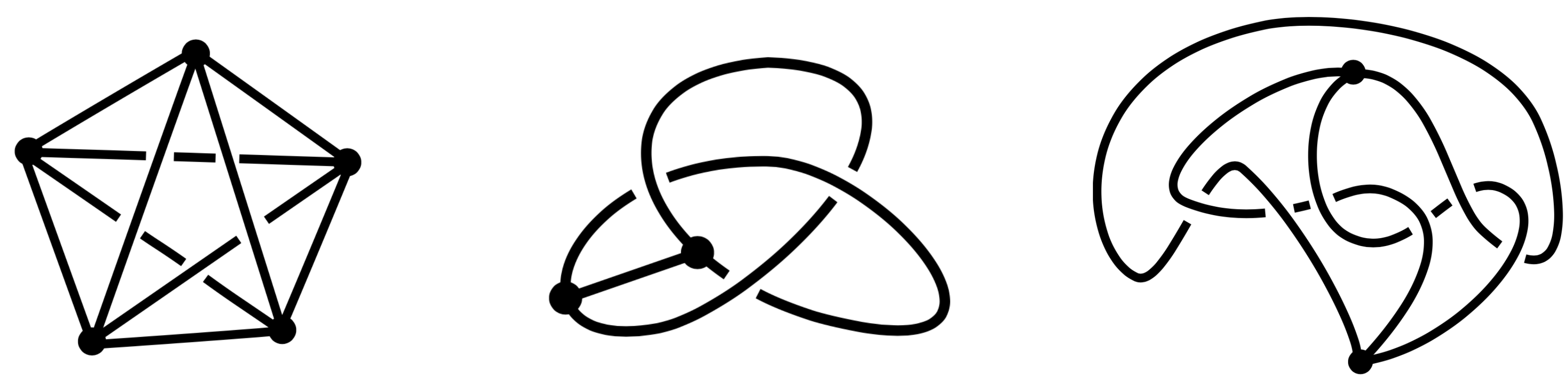
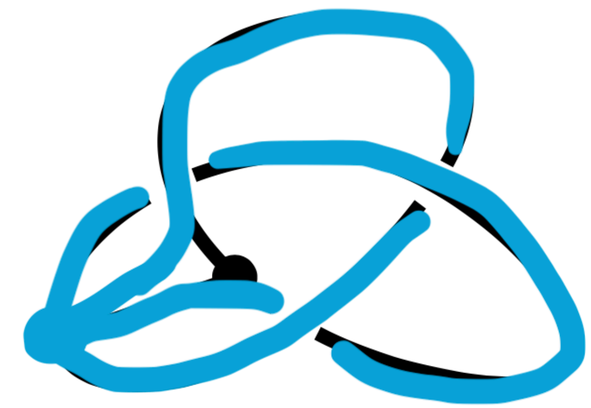


knotfree	✓	✗	✓
trivial	✗	✗	✗
(abstractly) planar	✗	✓	✓
panelled	✓	✗	✗
free			

Entanglements in spatial graphs



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	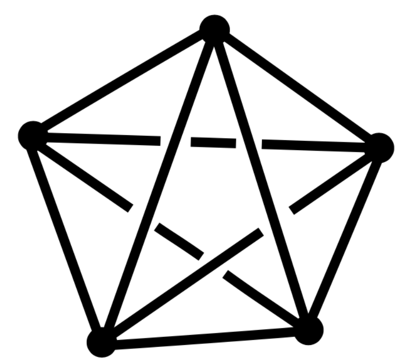	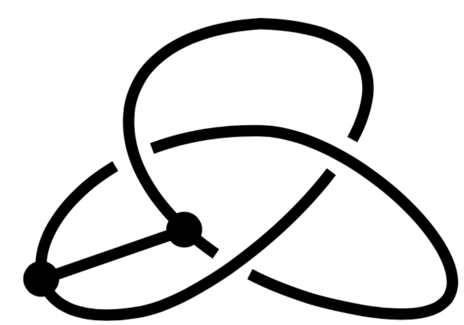	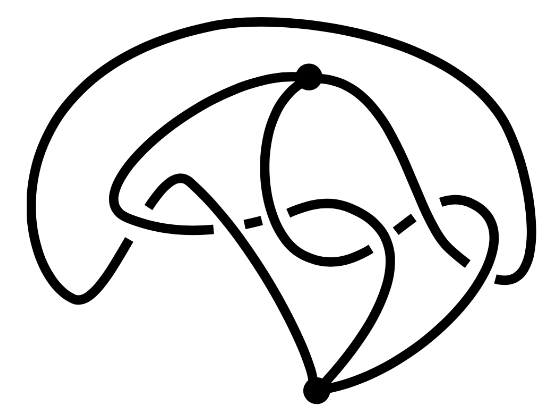
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trivial	✗	✗	✗
(abstractly) planar	✗	✓	✓
panelled	✓	✗	✗
free	✓		

Entanglements in spatial graphs

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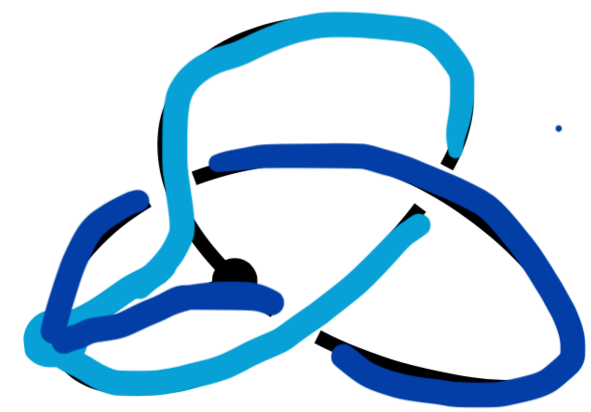

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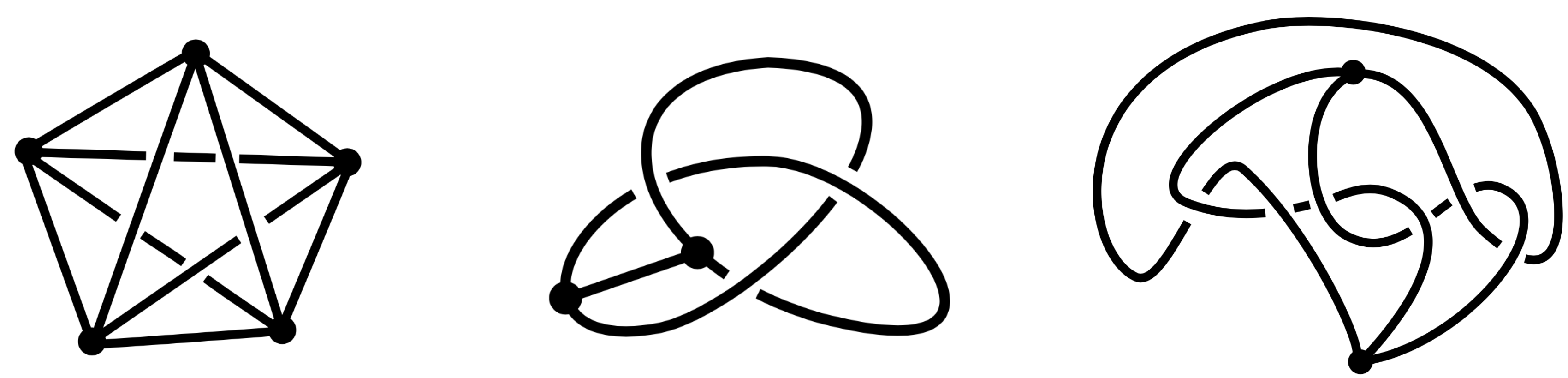

knotfree	✓	✗	✓
trivial	✗	✗	✗
(abstractly) planar	✗	✓	✓
panelled	✓	✗	✗
free	✓		

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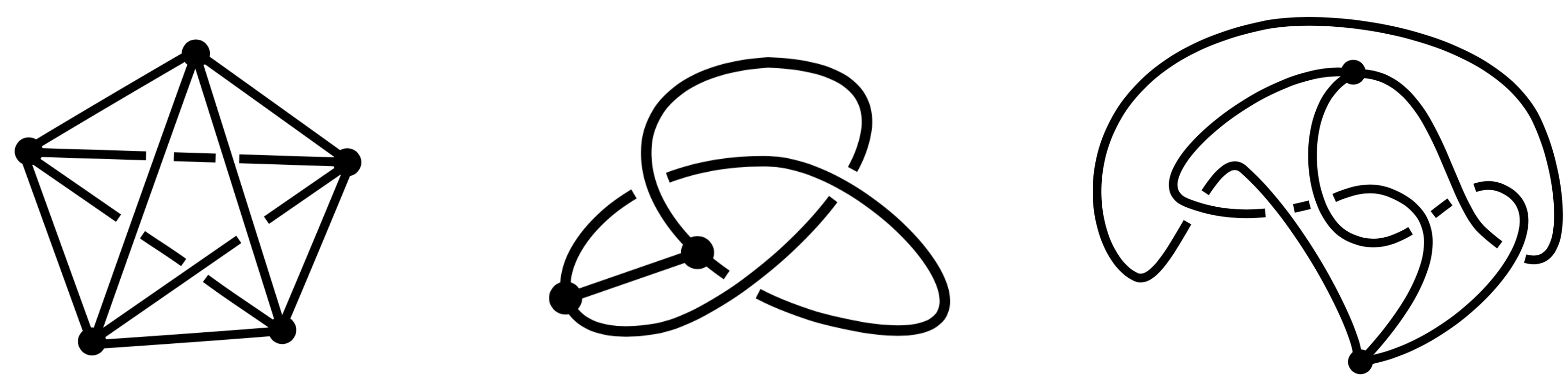
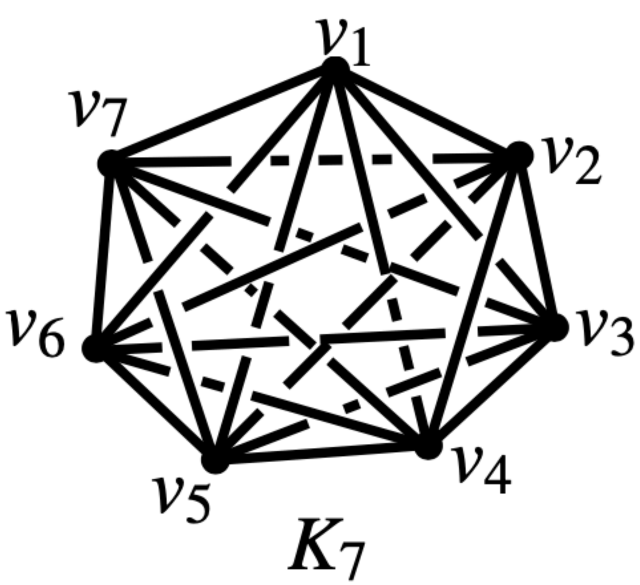
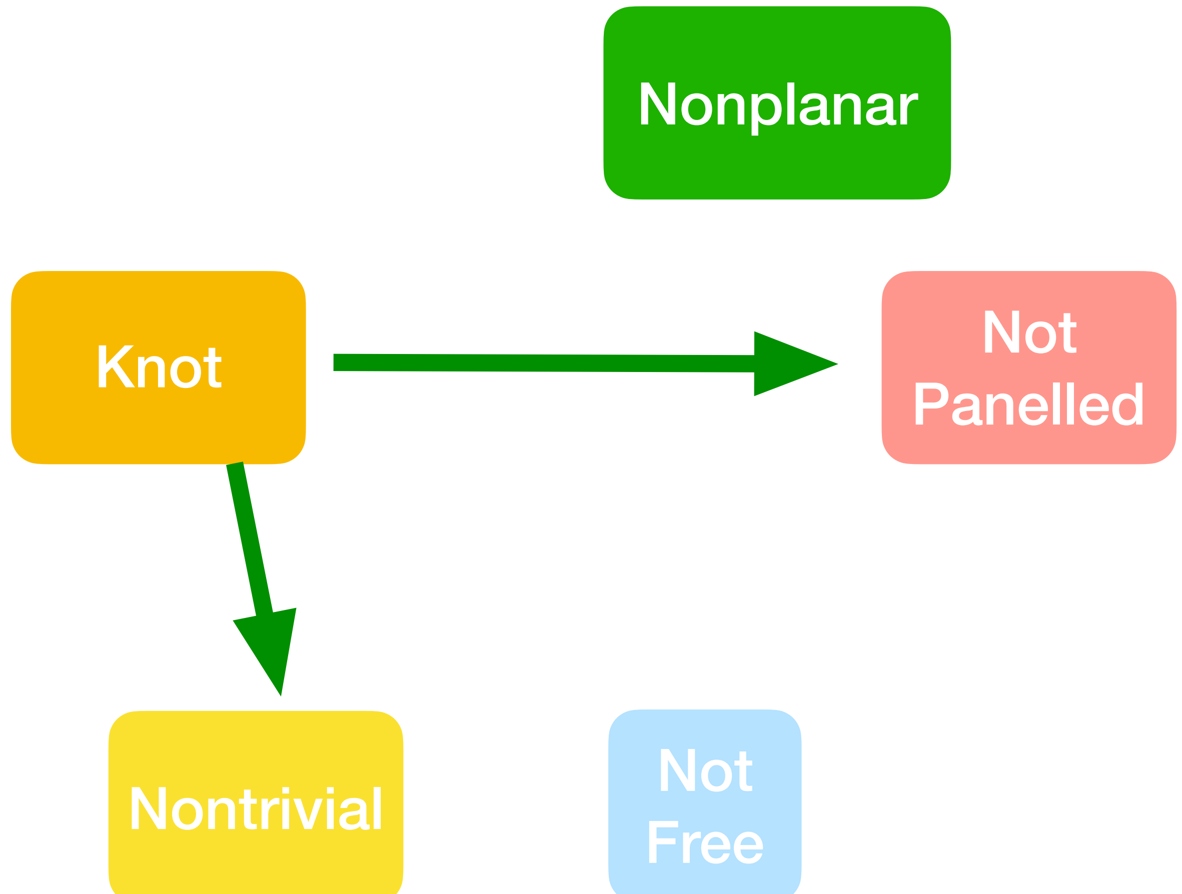


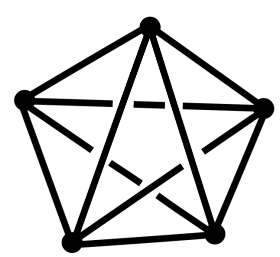
knotfree	✓	✗	✓
trivial	✗	✗	✗
(abstractly) planar	✗	✓	✓
panelled	✓	✗	✗
free	✓	✓	✗

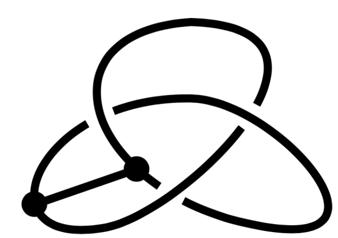
Relations of Entanglements

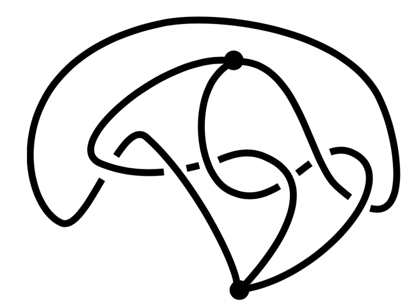
Intrinsically knotted:
Every embedding
contains a knot







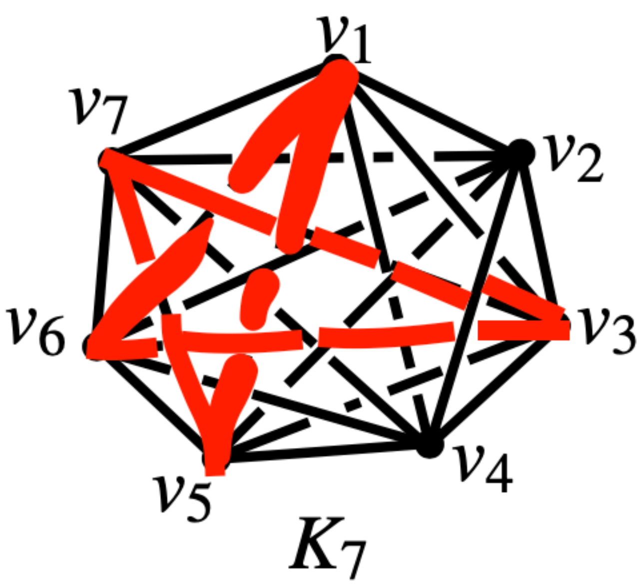


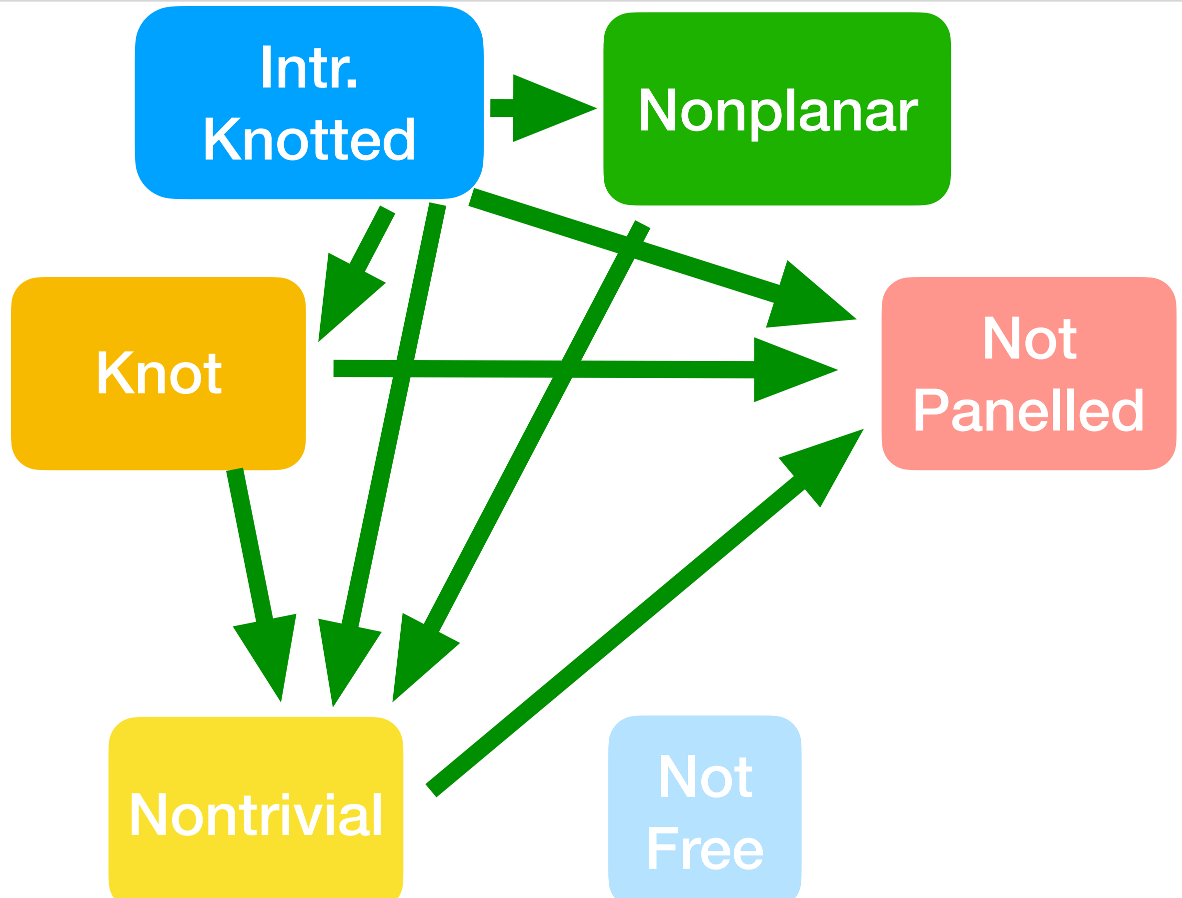


knot	✗	✓	✗
nontrivial	✓	✓	✓
(abstractly) nonplanar	✓	✗	✗
Not panelled	✗	✓	✓
Not free	✗	✗	✓

Relations of Entanglements

Intrinsically knotted: Every embedding contains a knot





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nontrivial	✓	✓	✓
(abstractly) nonplanar	✓	✗	✗
Not panelled	✗	✓	✓
Not free	✗	✗	✓

Relations of Entanglements

Theorem (Robertson, Seymour, Thomas):
$\mathcal{G}$ is panelled if and only if all its subgraphs $\mathcal{G}' \subseteq \mathcal{G}$ are free.

Theorem (Scharlemann, Thompson):
$\mathcal{G}$ is trivial

1) iff $\mathcal{G}$ is abstractly planar, free, and all proper subgraphs are trivial.
2) iff $\mathcal{G}$ is abstractly planar, and all subgraphs are free.
3) iff $\mathcal{G}$ is abstractly planar, ∂-reducible, and all proper subgraphs are free.

Theorem (Wu):
$\mathcal{G}$ is trivial

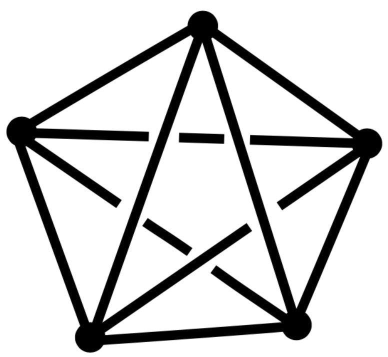
4) iff $\mathcal{G}$ is abstractly planar, and panelled.

More Entanglement Types

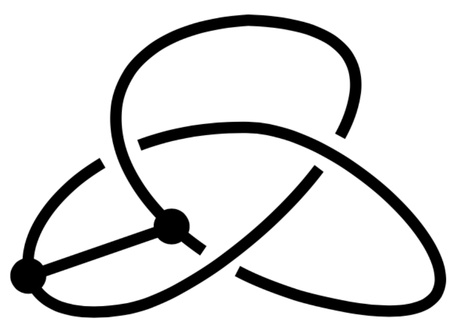
``Least entangled” (first after trivial):

- A spatial graph $\mathcal{G}$ is **minimal knotted** if
  $\mathcal{G}$ is nontrivial but for every edge e, both $\mathcal{G} \setminus e$ and $\mathcal{G} - e$ are trivial.

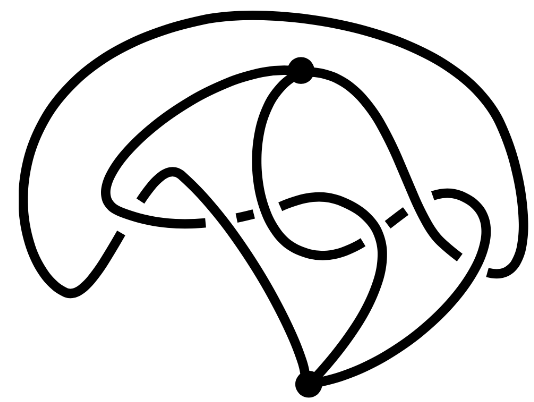
- Embeds on the standard torus but is not trivial.



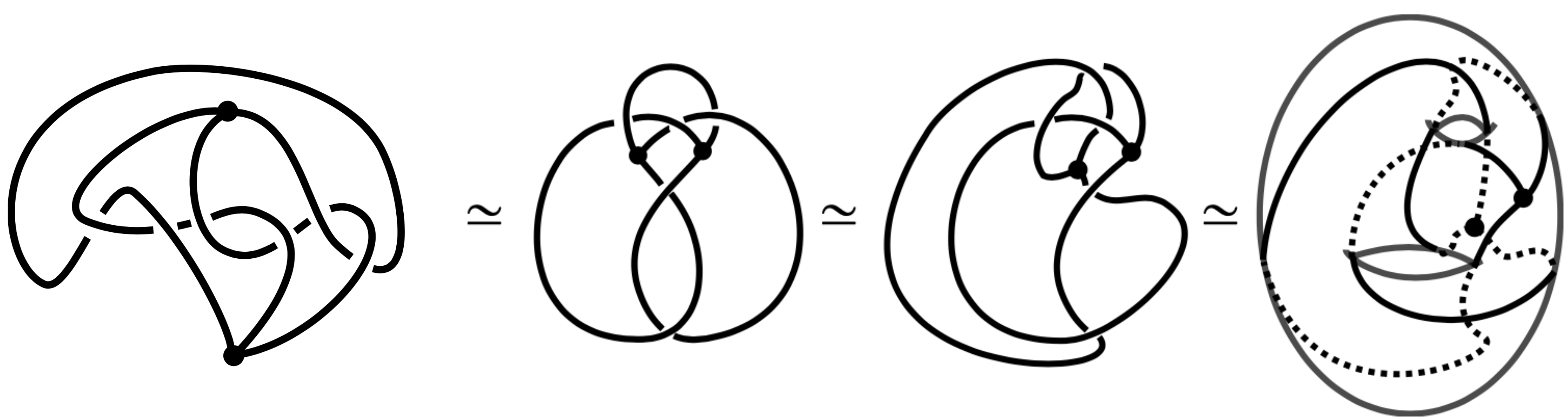
minimal knotted on torus



not minimal knotted on torus



minimal knotted on genus 2 surface



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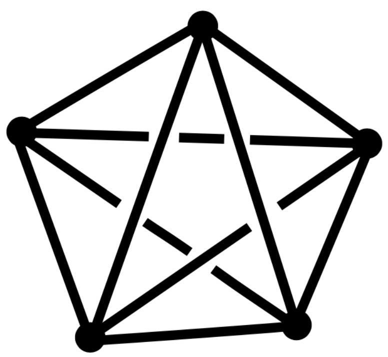
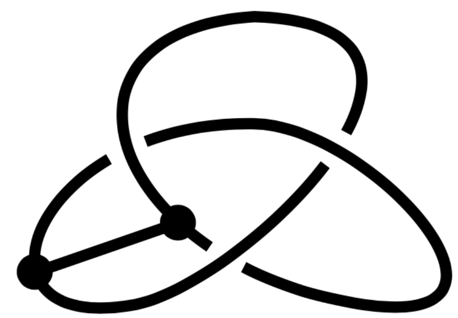
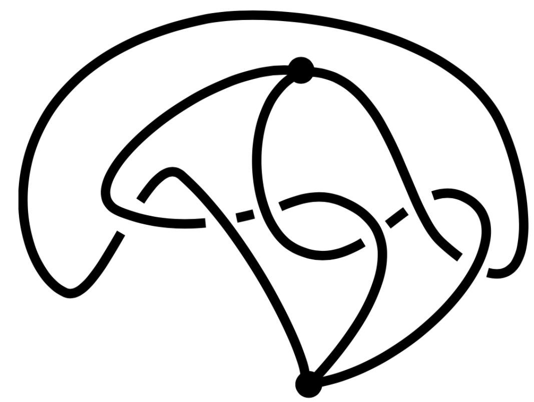


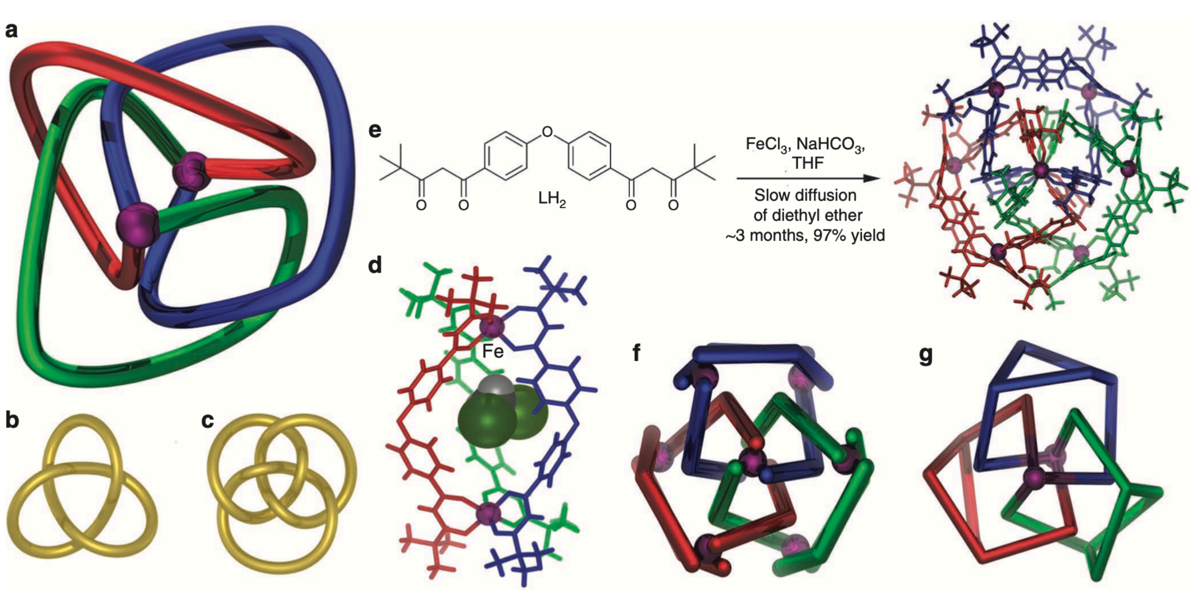
minimal knotted on torus

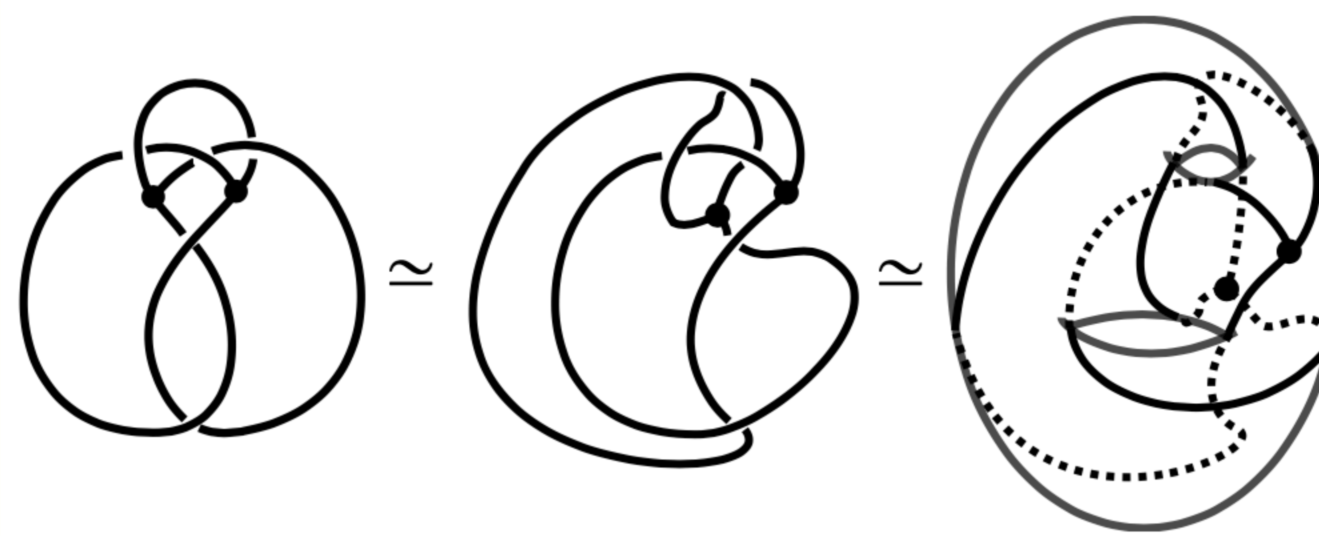


not minimal knotted on torus



minimal knotted on genus 2 surface





More Entanglement Types

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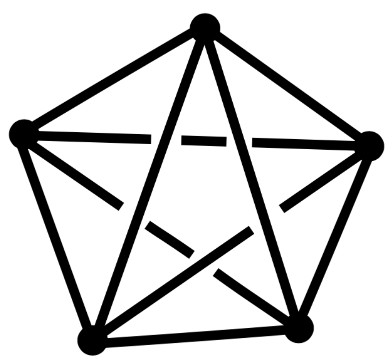
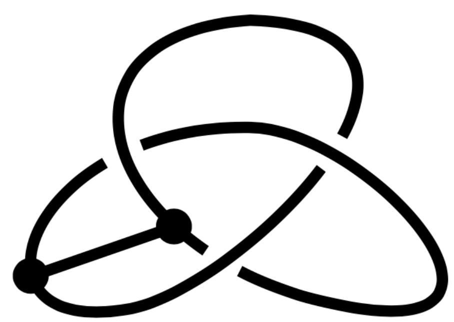
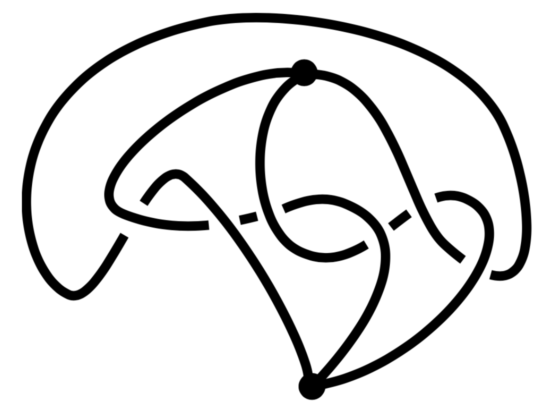


minimal knotted on torus



not minimal knotted on torus



minimal knotted on genus 2 surface

Remark:

Minimal knotted graphs do not contain proper subgraphs that are knotted or linked.

Minimally knotted abstractly planar spatial graphs are not panelled.

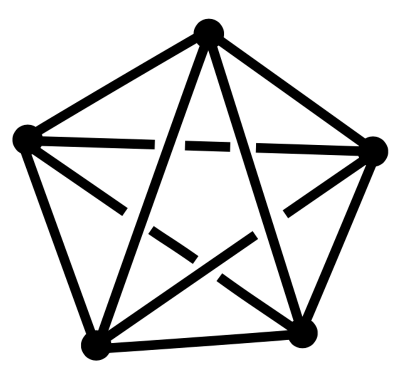
Minimally knotted abstractly planar graphs are not free.

Entanglements on the Torus

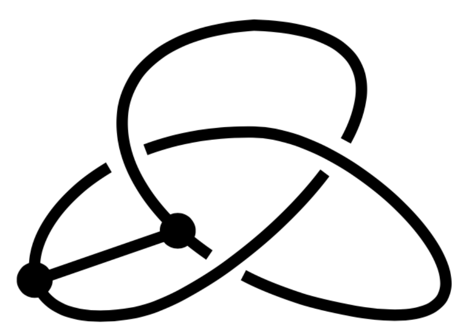
Theorem (B)**:**
If an abstractly planar spatial graph is nontrivially embedded on the torus, it contains a nontrivially knotted or linked subgraph.

Reformulation:
`Stabilising' a nontrivial embedding of an abstractly planar graph on the torus can only be done by introducing a nontrivial knot or link.

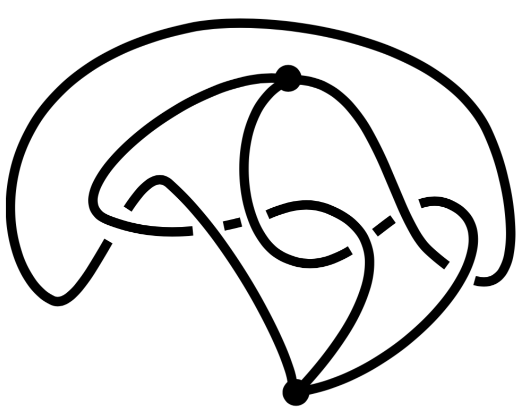
Consequence:
Let G be a graph that it is not a subdivision of a circle.
Then a minimally knotted embedding of G embeds one a surface of genus at least two.



minimal knotted
on torus
nonplanar



not minimal knotted
on torus
planar



minimal knotted
on genus 2 surface
planar

Entanglements on the Torus

Theorem (B)**:**
If an abstractly planar spatial graph is nontrivially embedded on the torus,
it contains a nontrivially knotted or linked subgraph.

Idea of the proof:
Let $\mathcal{G}$ be a knot-free and link-free embedding on the torus of a planar graph G.
We show that it follows that $\mathcal{G}$ is trivial.

1. Statement is true for non-standardly embedded tori
2. It is sufficient to restrict to connected graphs
3. A bouquet graph on T^2 either contains a nontrivial knot or is trivial

Combining:
Any connected graph G on T^2 contracts to a bouquet graph on T^2
$\Rightarrow$ the bouquet is trivial, all connected subgraphs of $\mathcal{G}$ are free
$\Rightarrow$ $\mathcal{G}$ is trivial (by theorem of Scharlemann and Thompson) ■

Thank you!

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