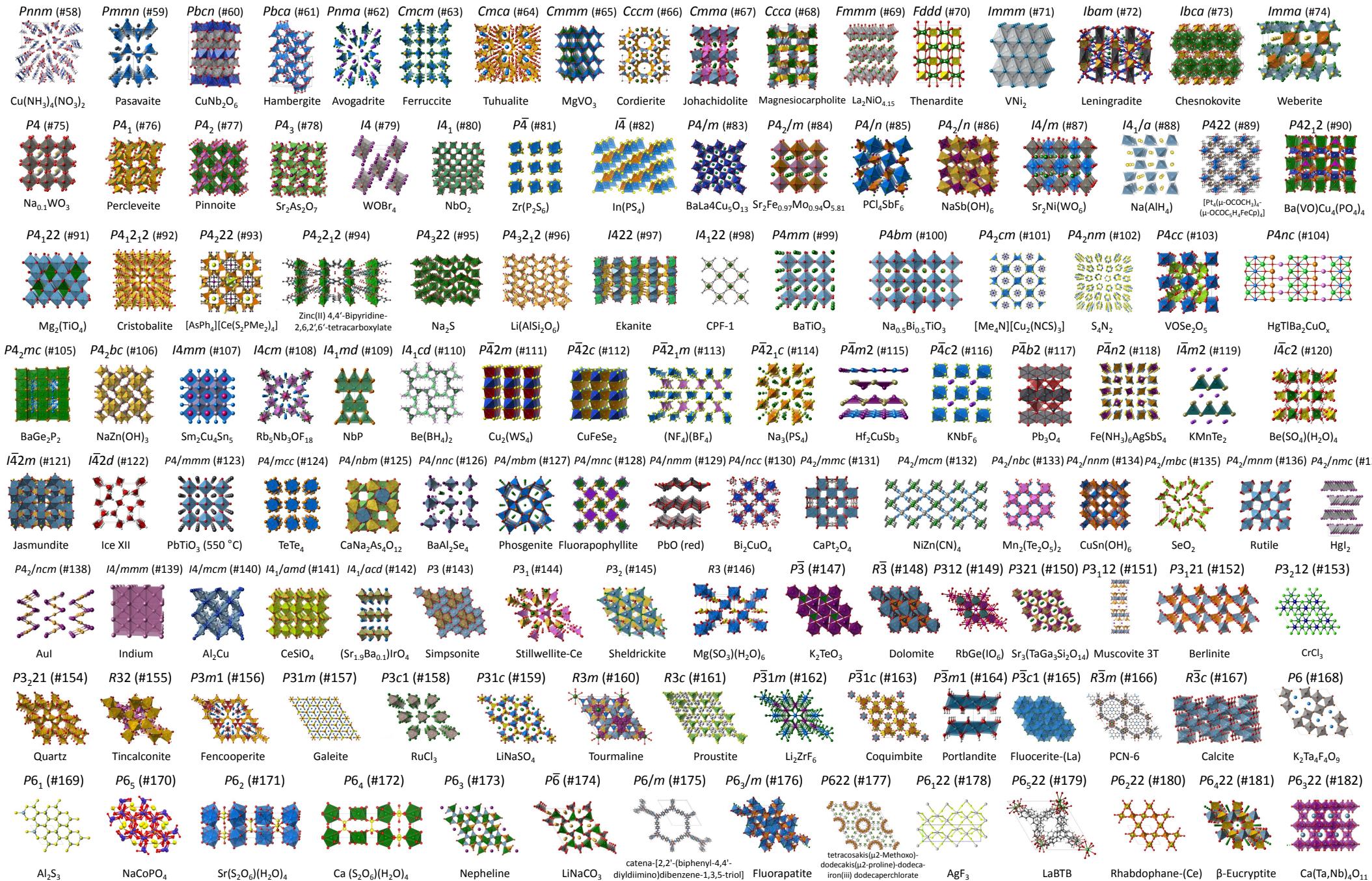


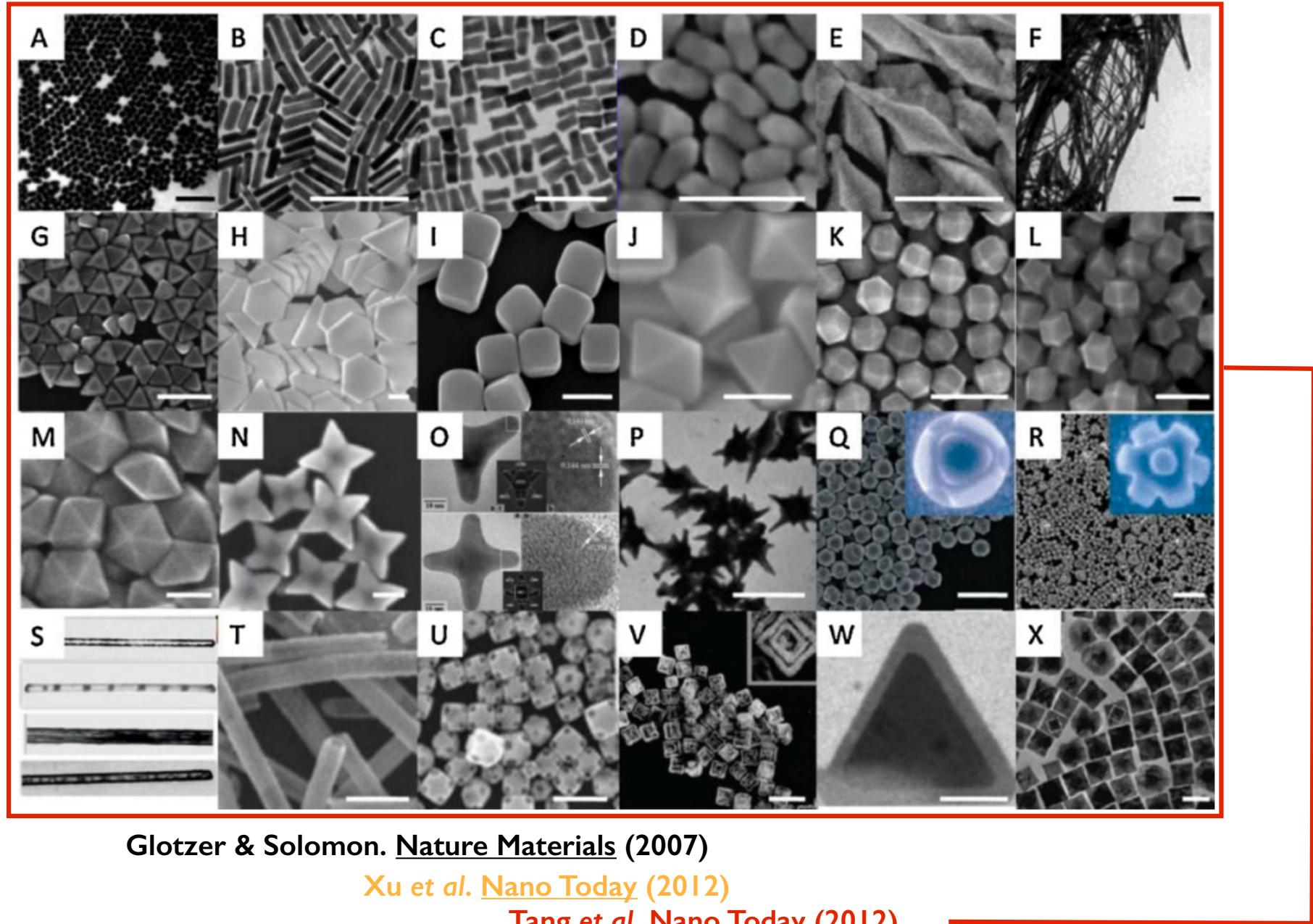
Self-Assembly of Complex Crystals Through Building Block Design

Pablo F. Damasceno, UCSF

What do I mean by complex crystal structures?

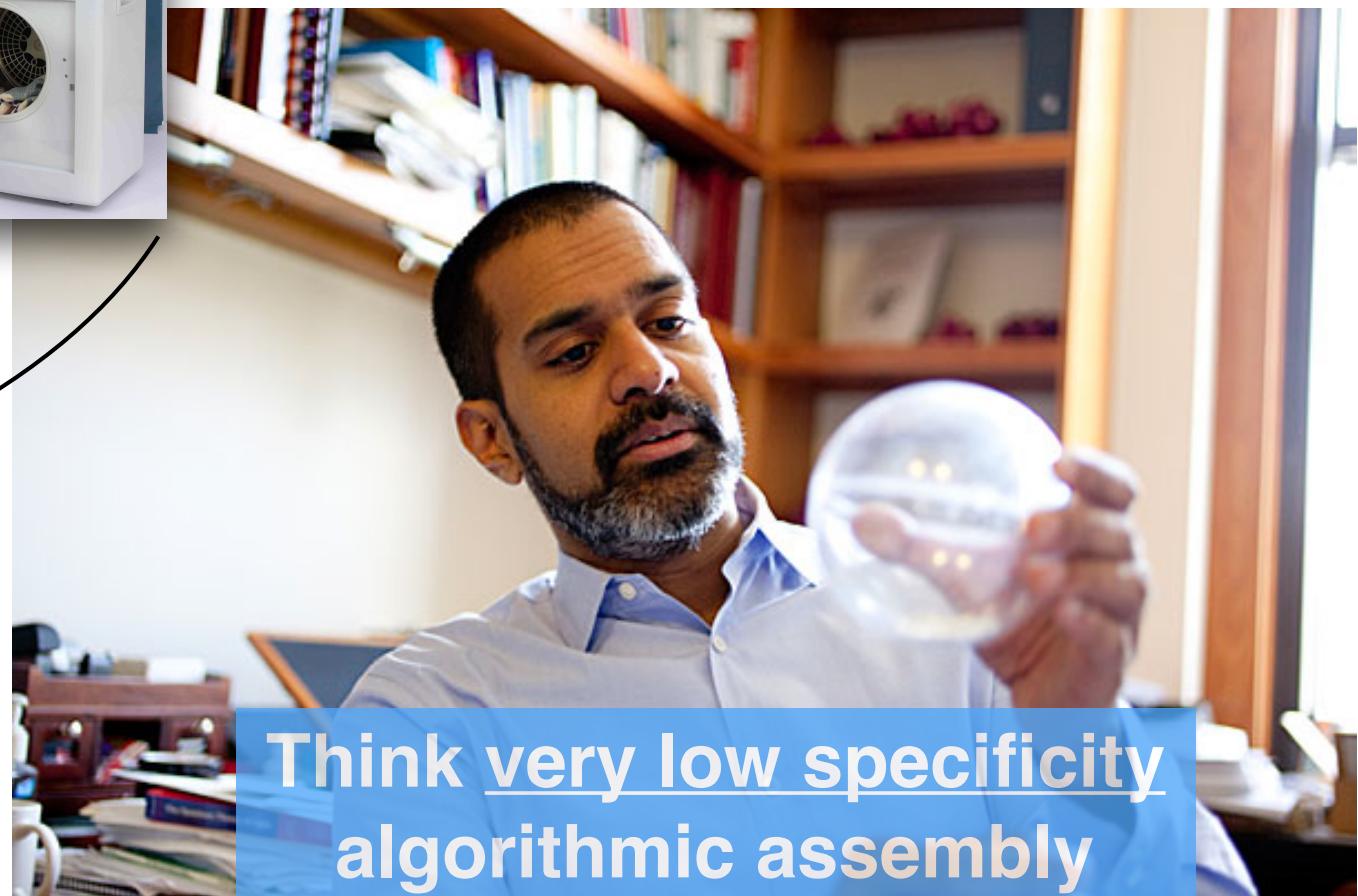
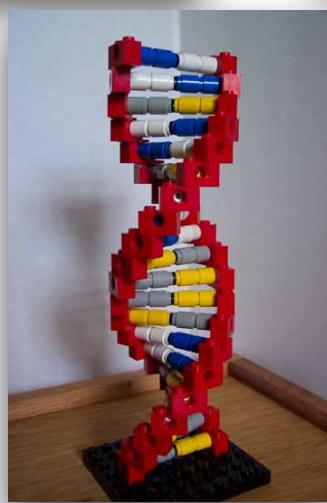


Building Block Design



Self-Assembling Crystal Structures

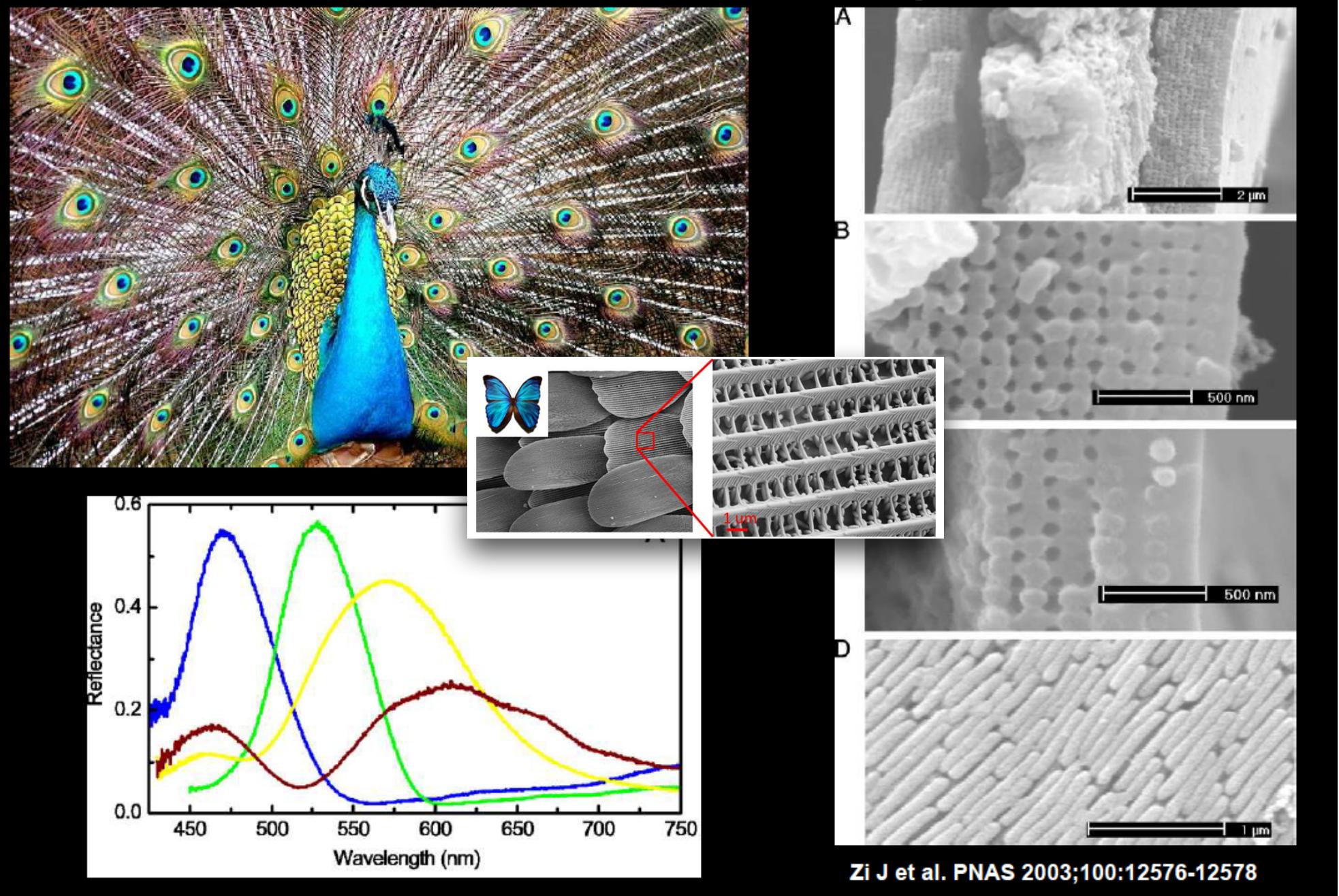
“Imagine gently shaking a box of Lego building blocks, and then looking inside to find a series of complete structures.”



Think very low specificity
algorithmic assembly

Vinothan Manoharan

One Application: Photonic Materials



Questions

1. What is the role of *shape* for the self-assembly of complex structures?

Damasceno, Engel & Glotzer. **Science** (2012)

2. What is the information *cost* for assembling a complex crystal?

- Is it *harder* to assemble a crystal with large unit cell ?

Engel, Damasceno, Phillips & Glotzer. **Nature Materials** (2014)

- Can we predict what will be assembled from generic rules?

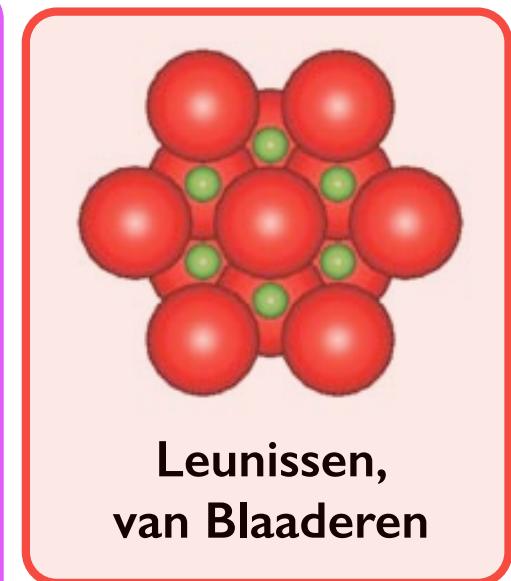
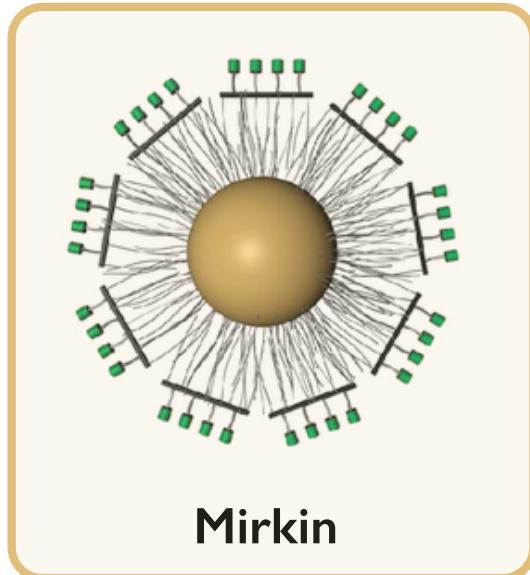
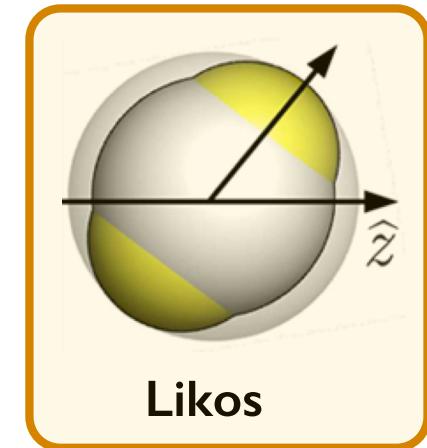
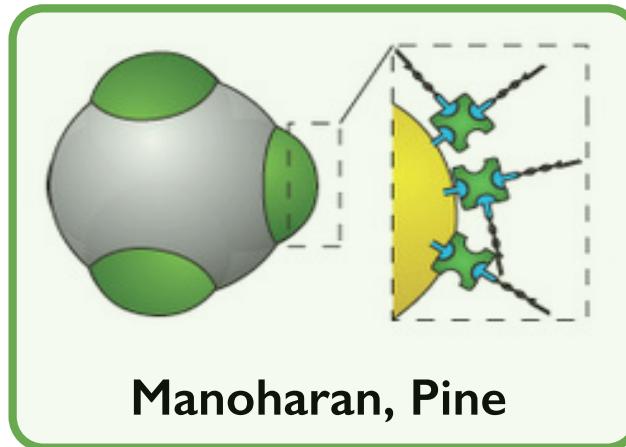
Damasceno, Engel & Glotzer. **ACS Nano** (2012)

3. Can we reverse engineer building blocks for target assembly?

Damasceno, Karas, Schultz, Engel & Glotzer. **PRL** (2015)

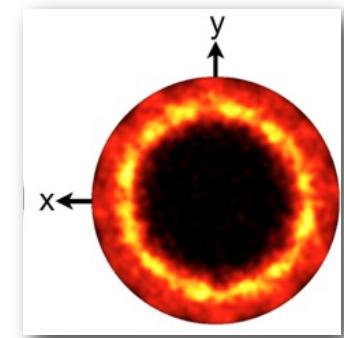
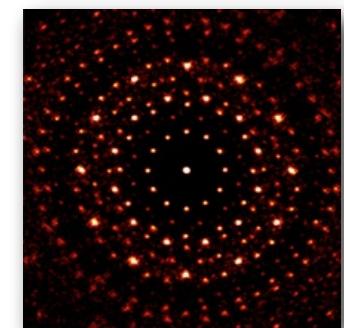
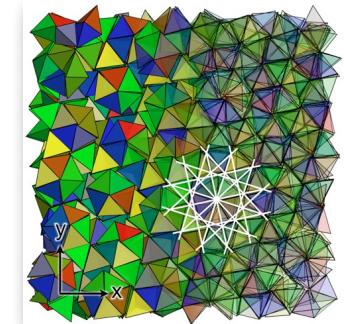
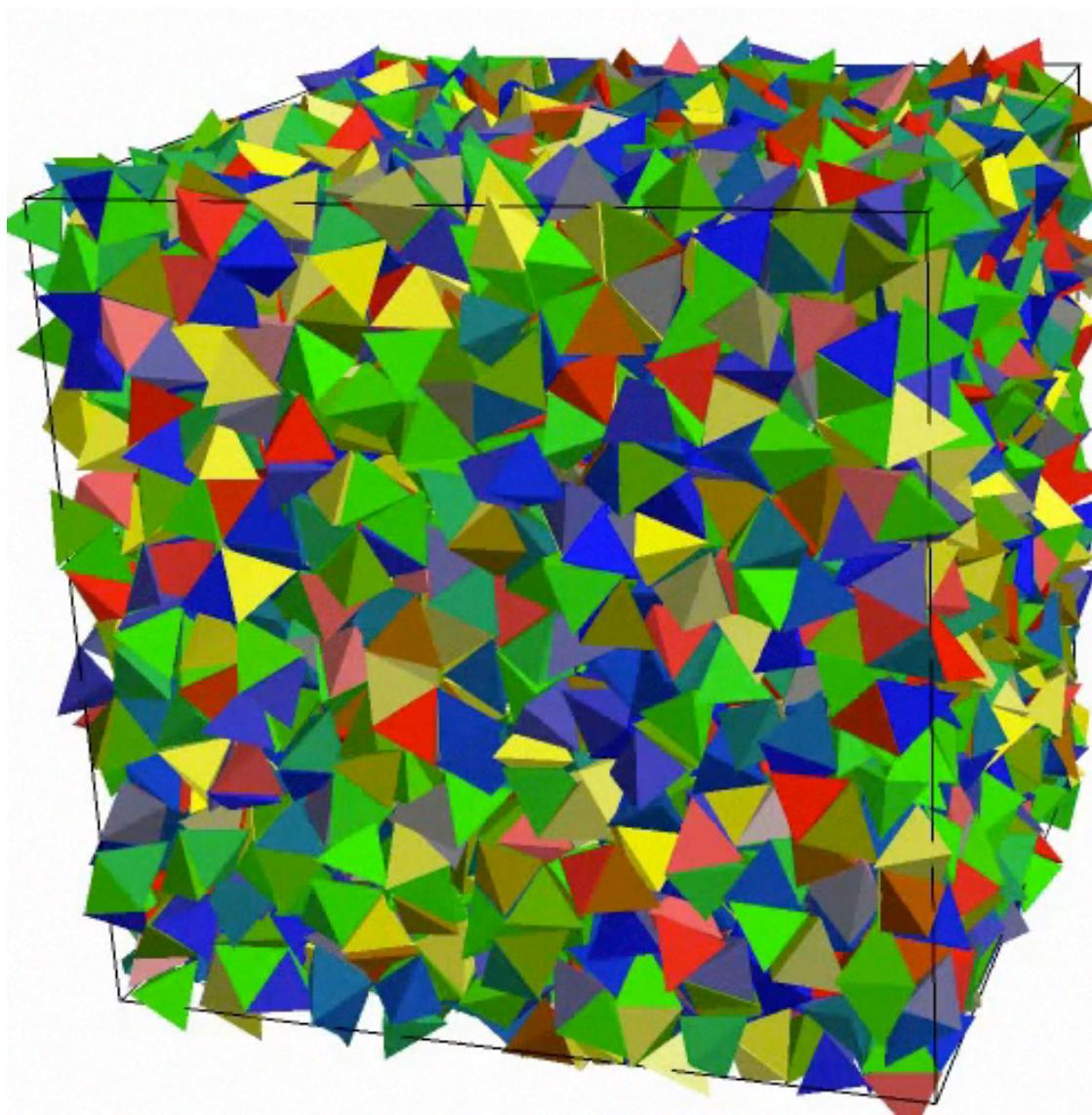
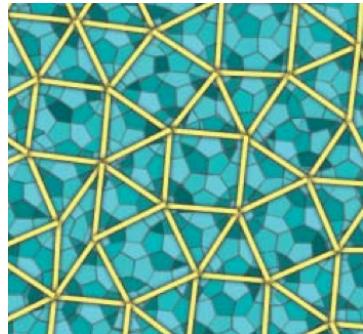
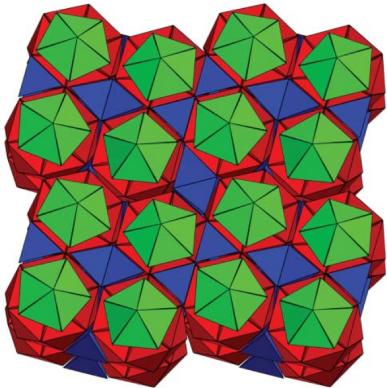
Cadotte, Dshemuchadse, Damasceno, Newman & Glotzer. **Soft Matter** (2016)

Role of shape (directionality) for SA



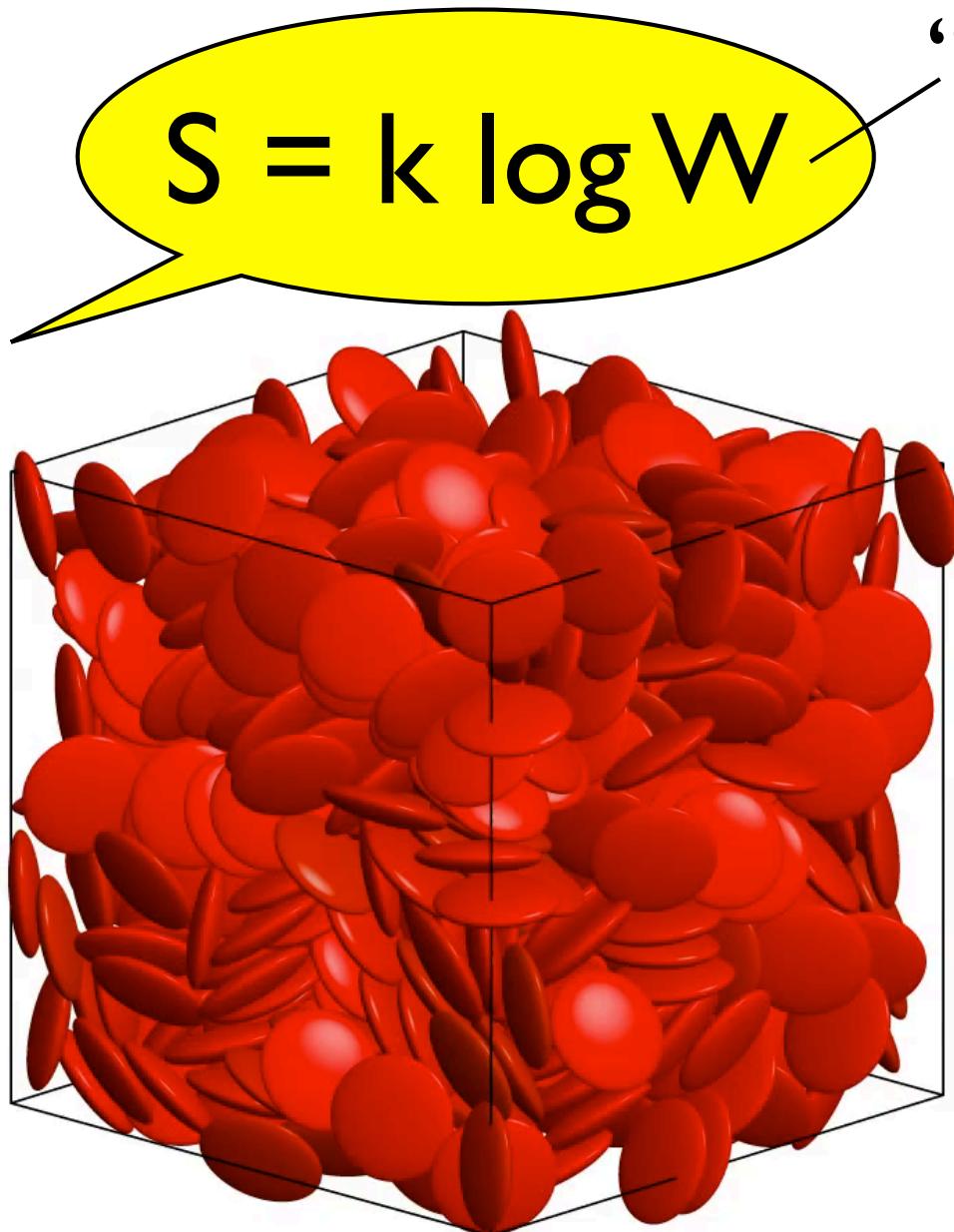
Strategy: Monte Carlo Simulations

Task: Isolate the effect of particle shape for self-assembly

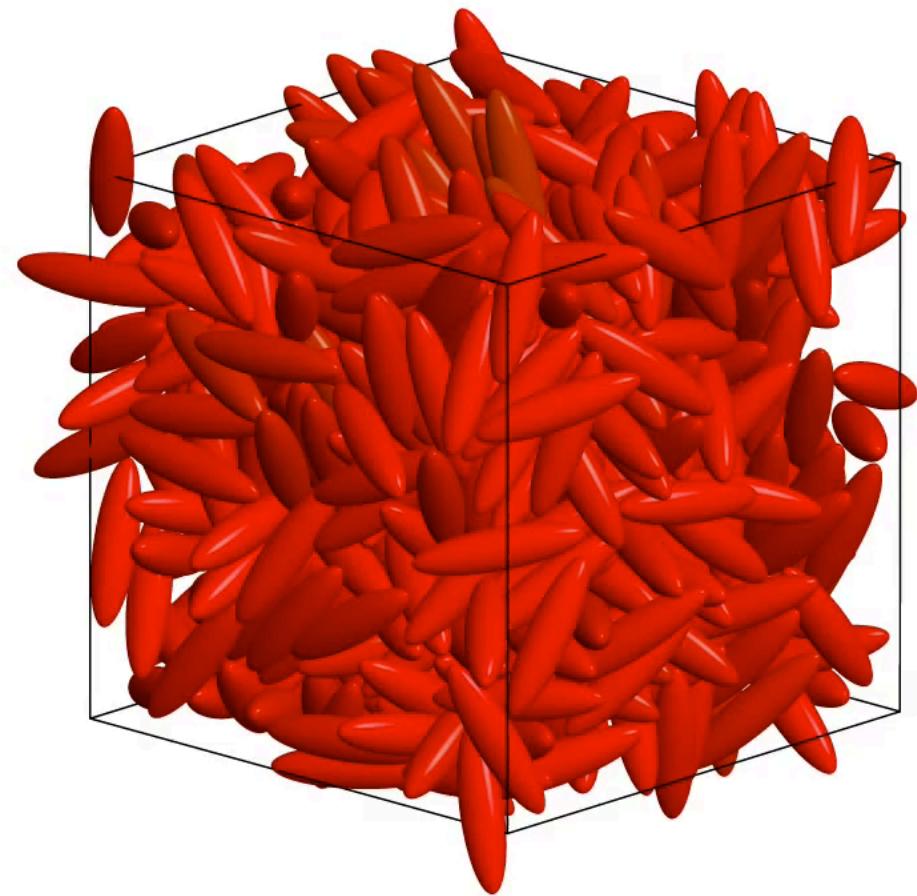


A. Haji-Akbari, M. Engel, A.S. Keys, X.Y. Zhang, R.G. Petschek, P. Pálffy-Muhoray, S.C. Glotzer, *Nature*, 462, 773 (2009)

Entropic Order

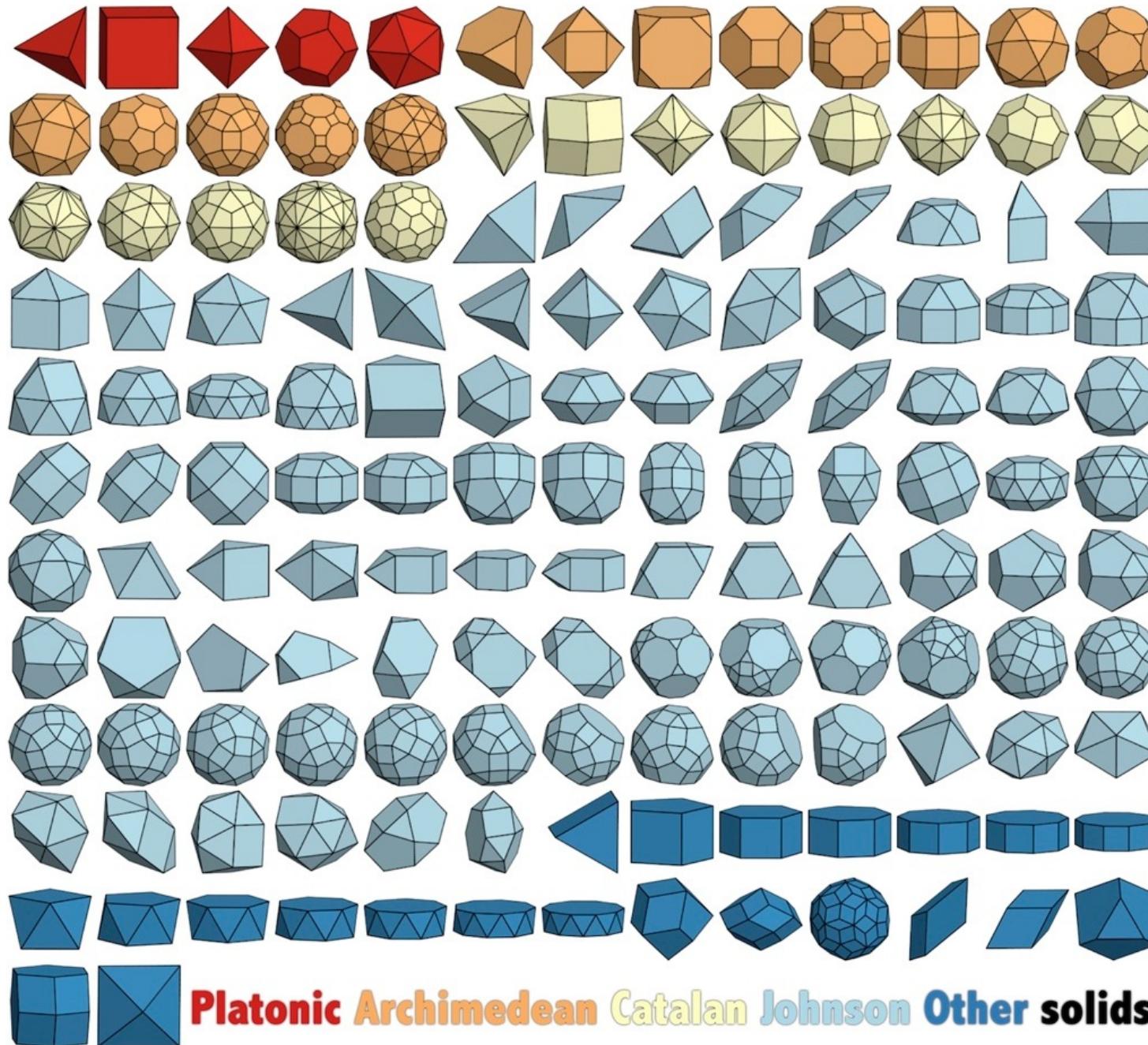


“Ways”

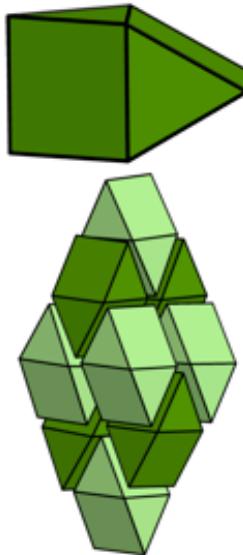
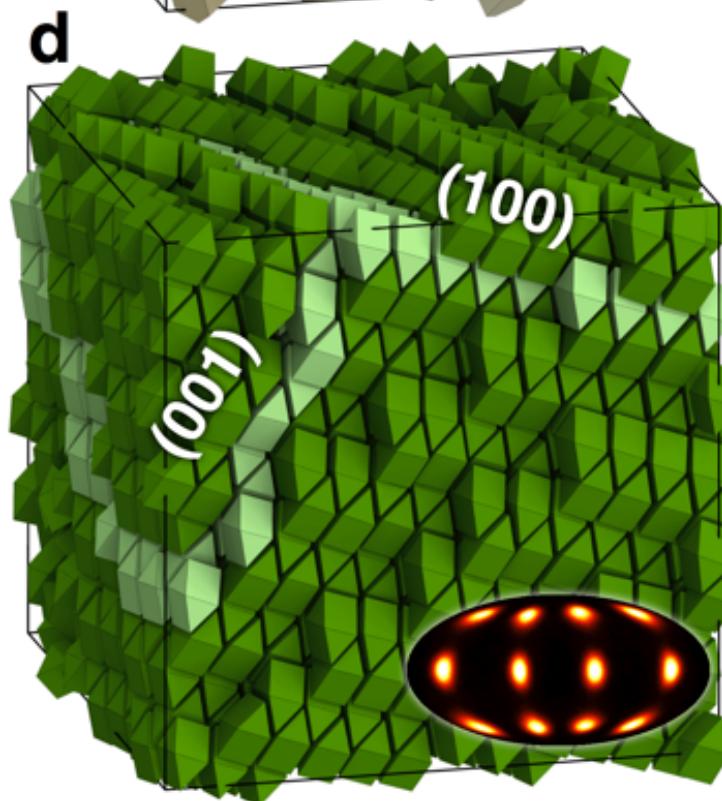
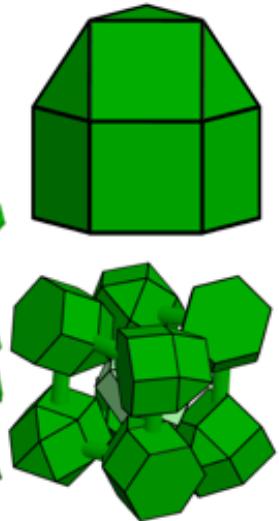
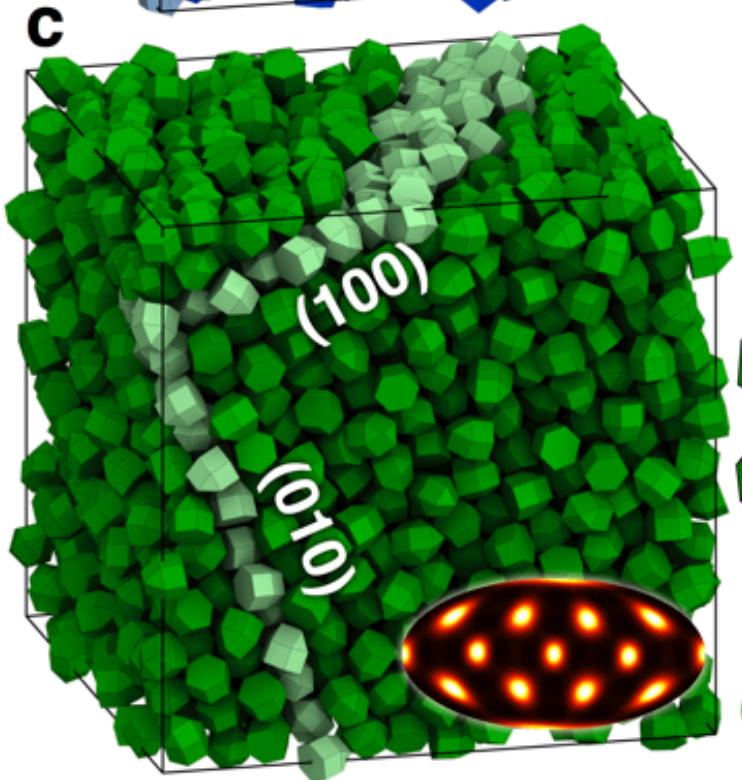
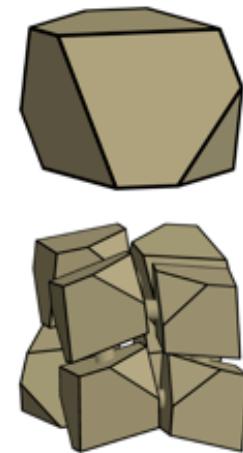
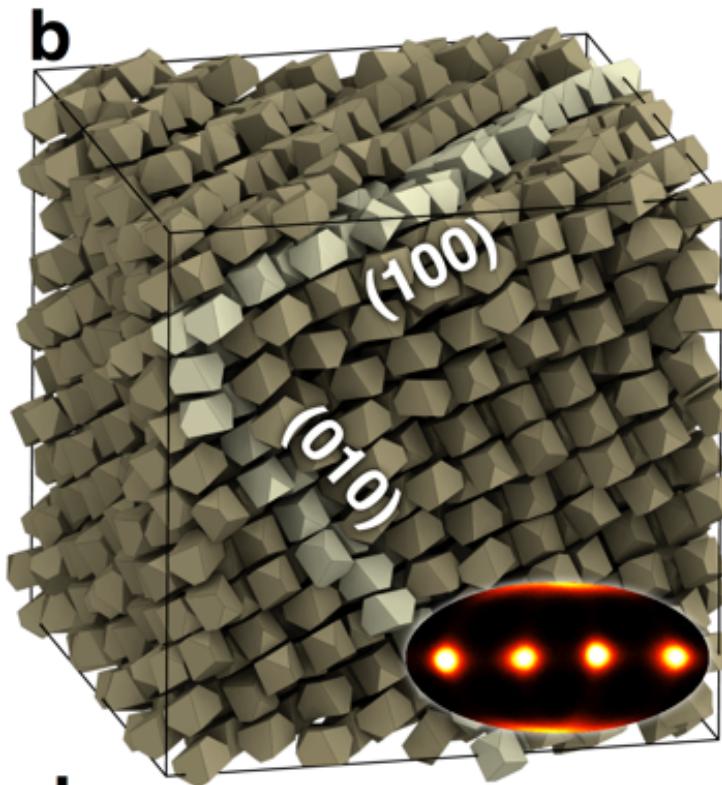
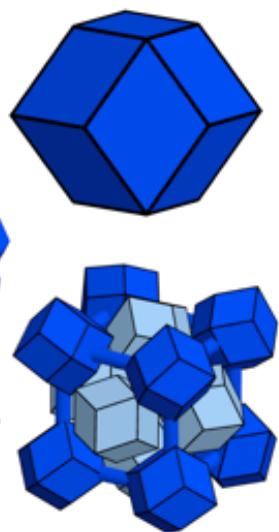
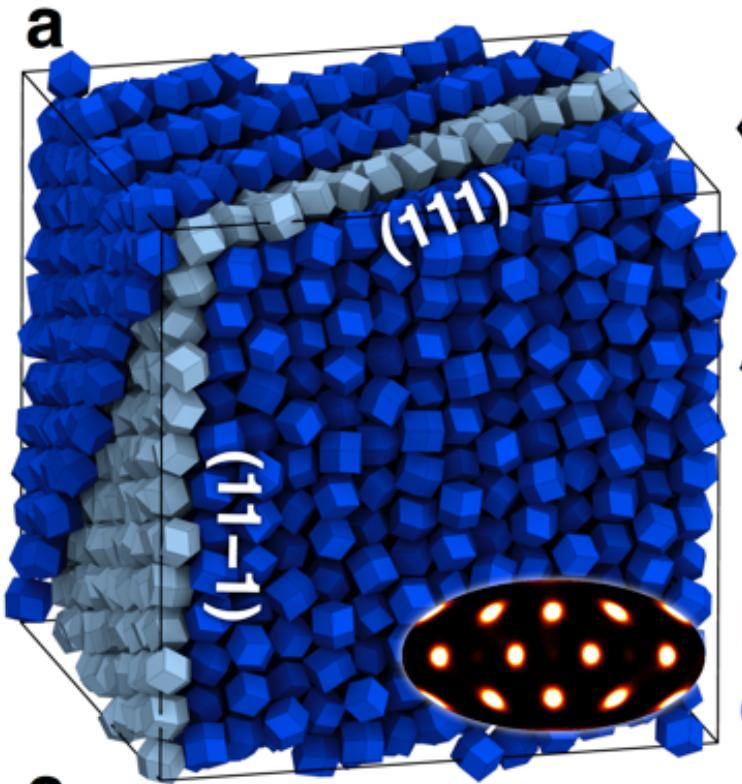


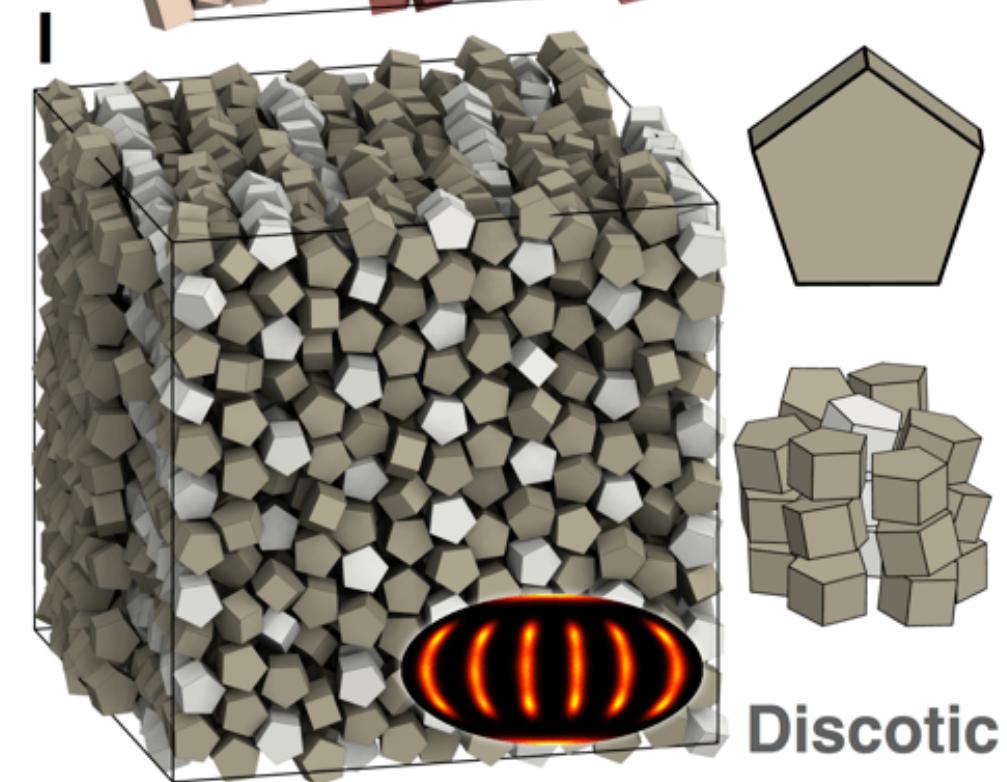
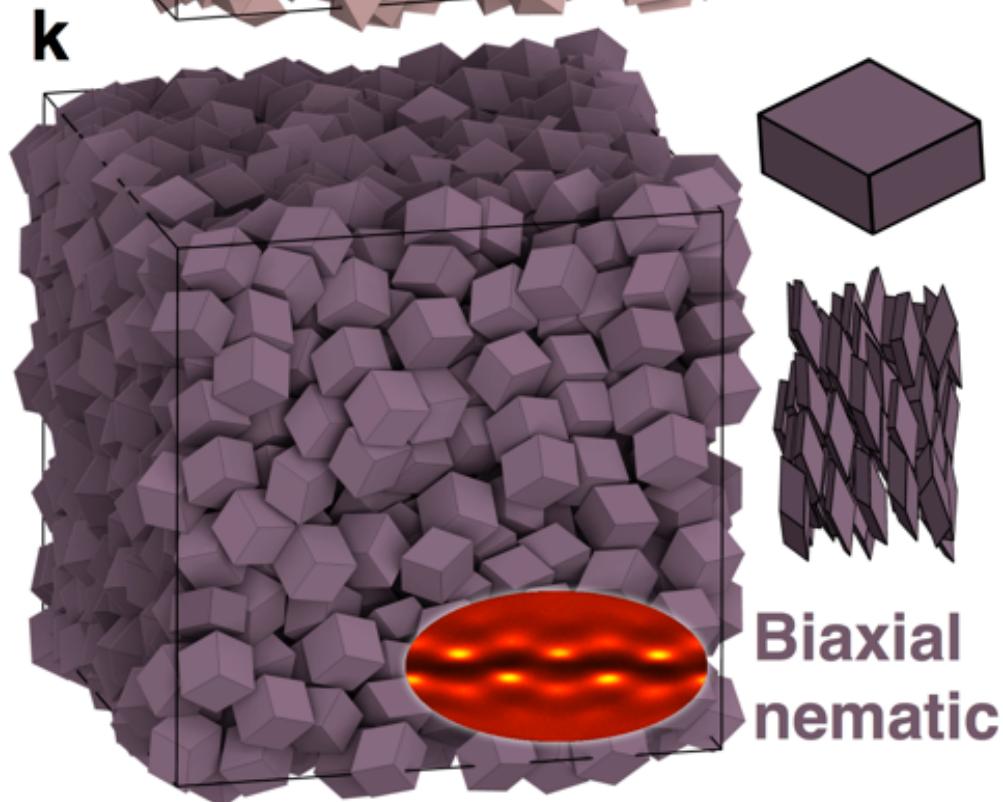
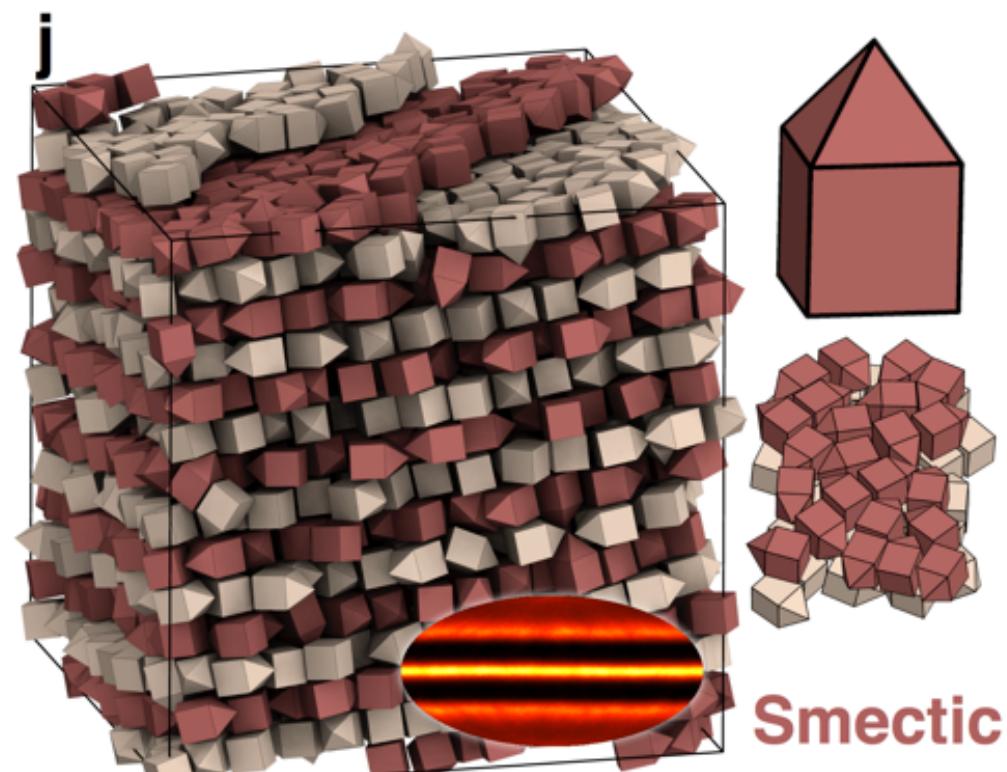
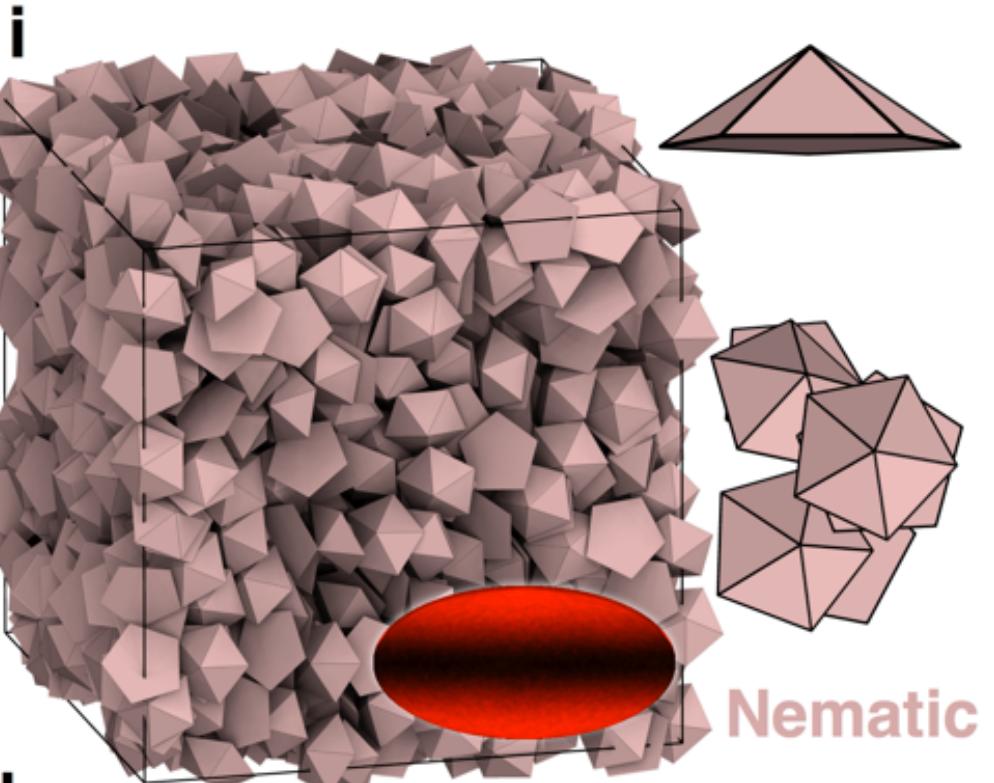
$$F = U - TS + pV$$
$$\partial F = -T\partial S$$

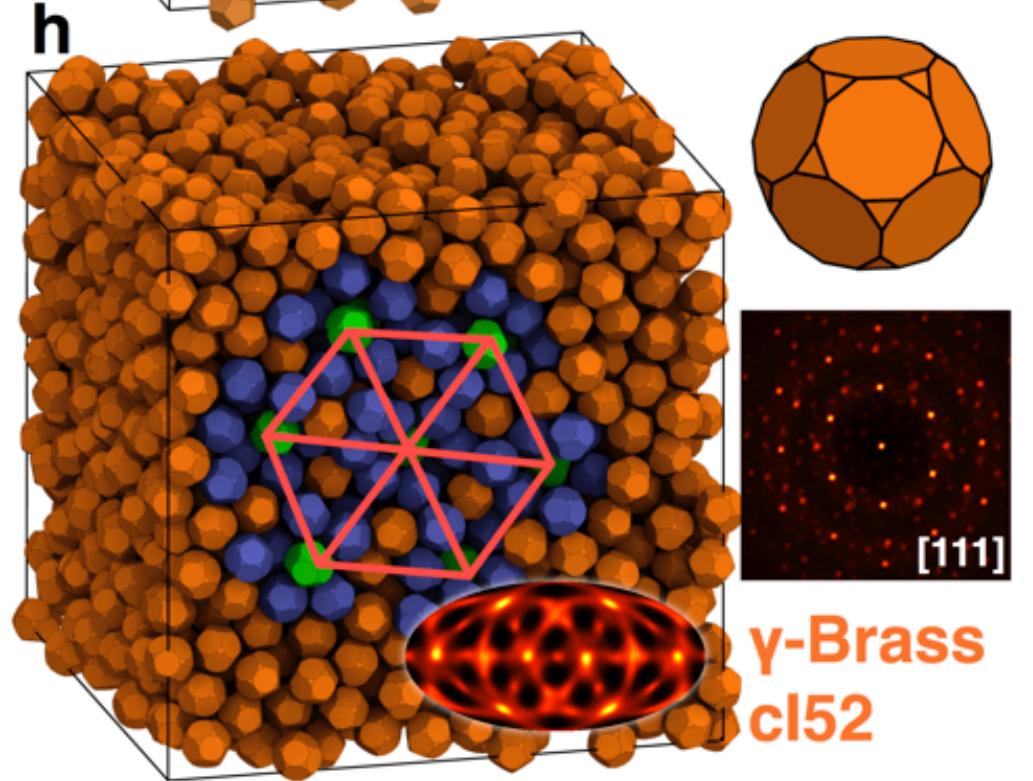
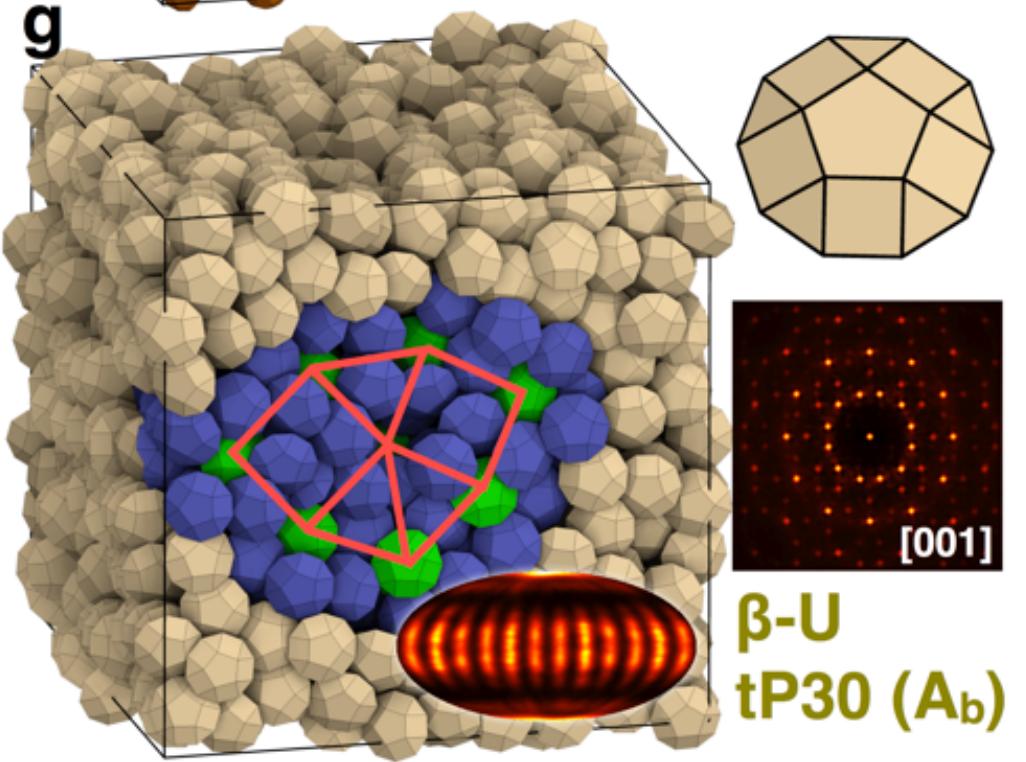
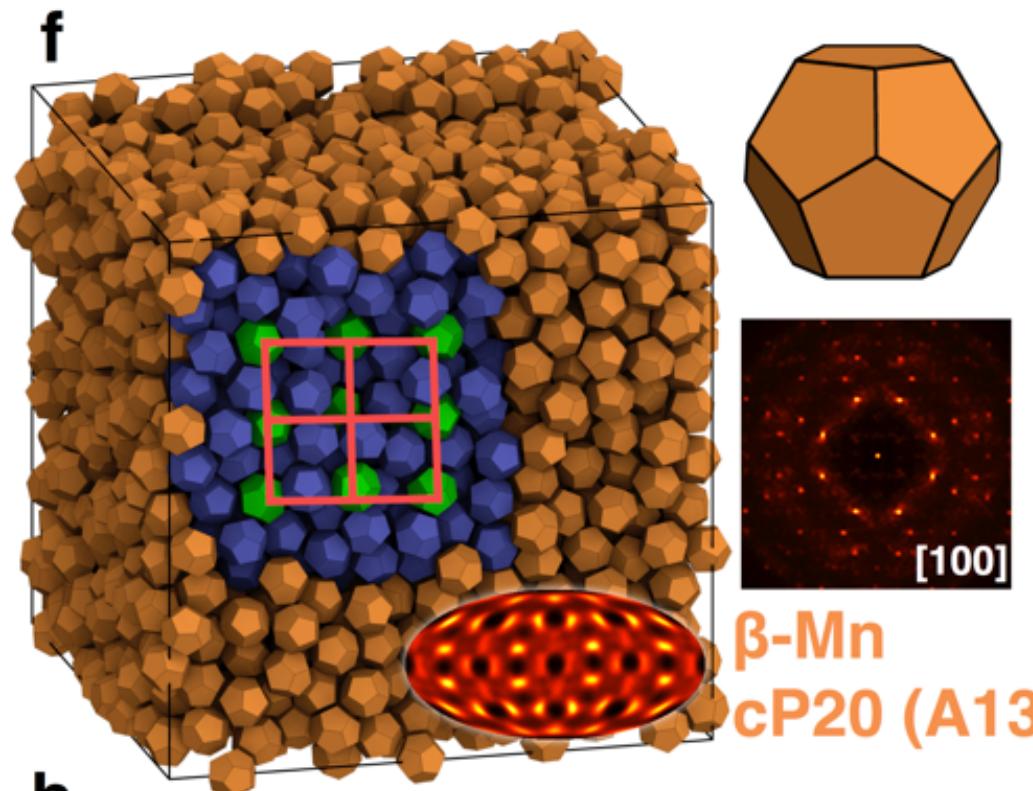
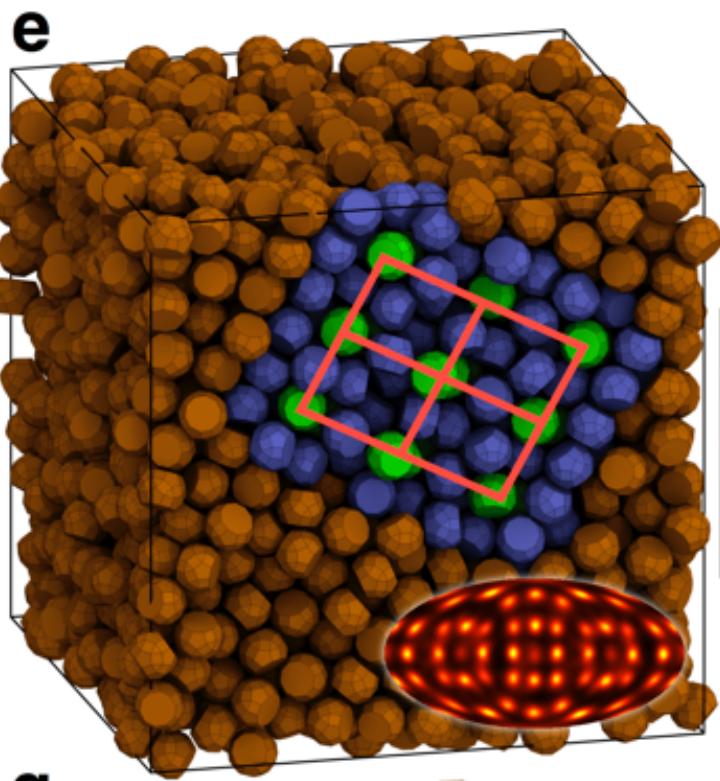
Would it work for other shapes ?

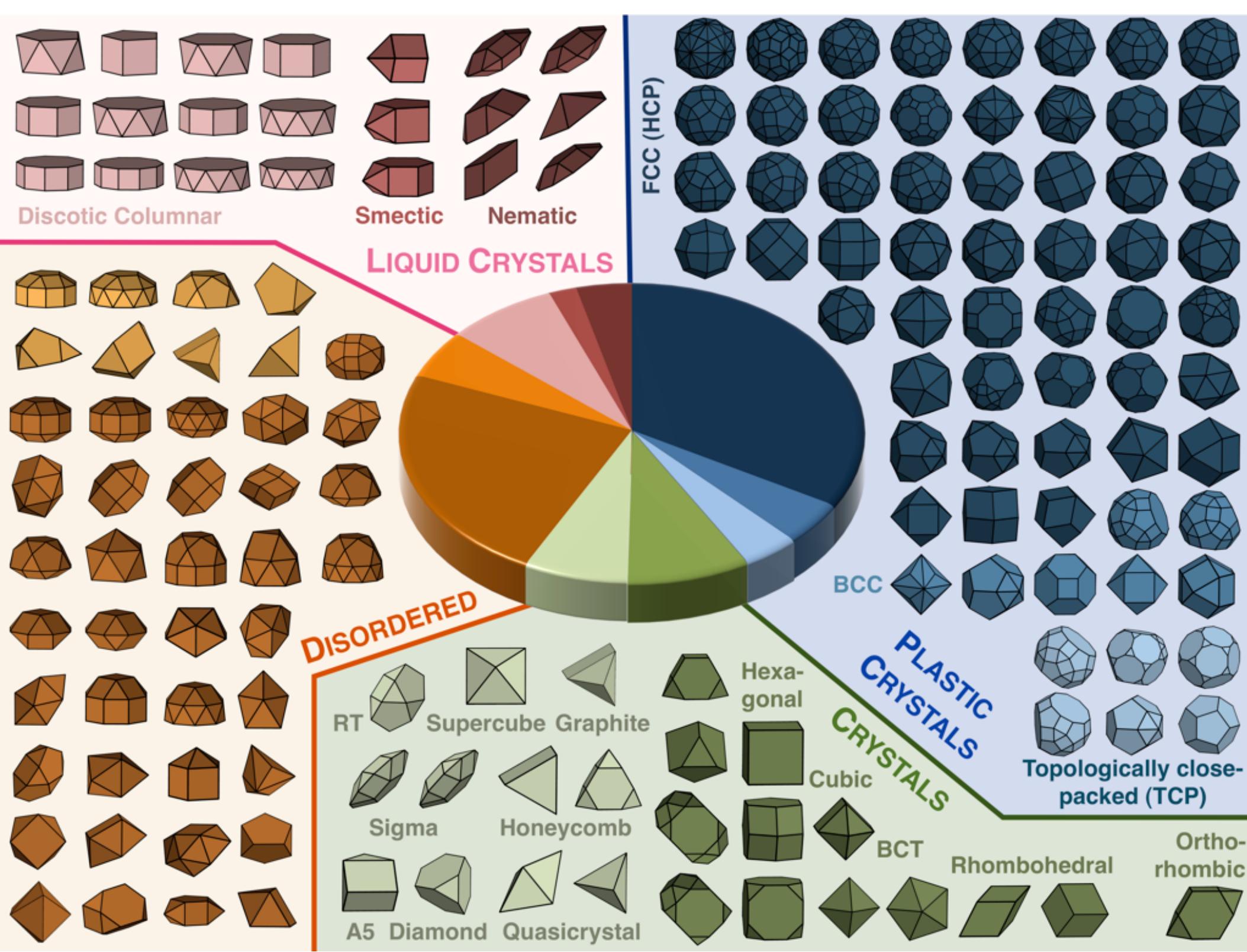


Platonic **Archimedean** **Catalan** **Johnson** **Other solids**

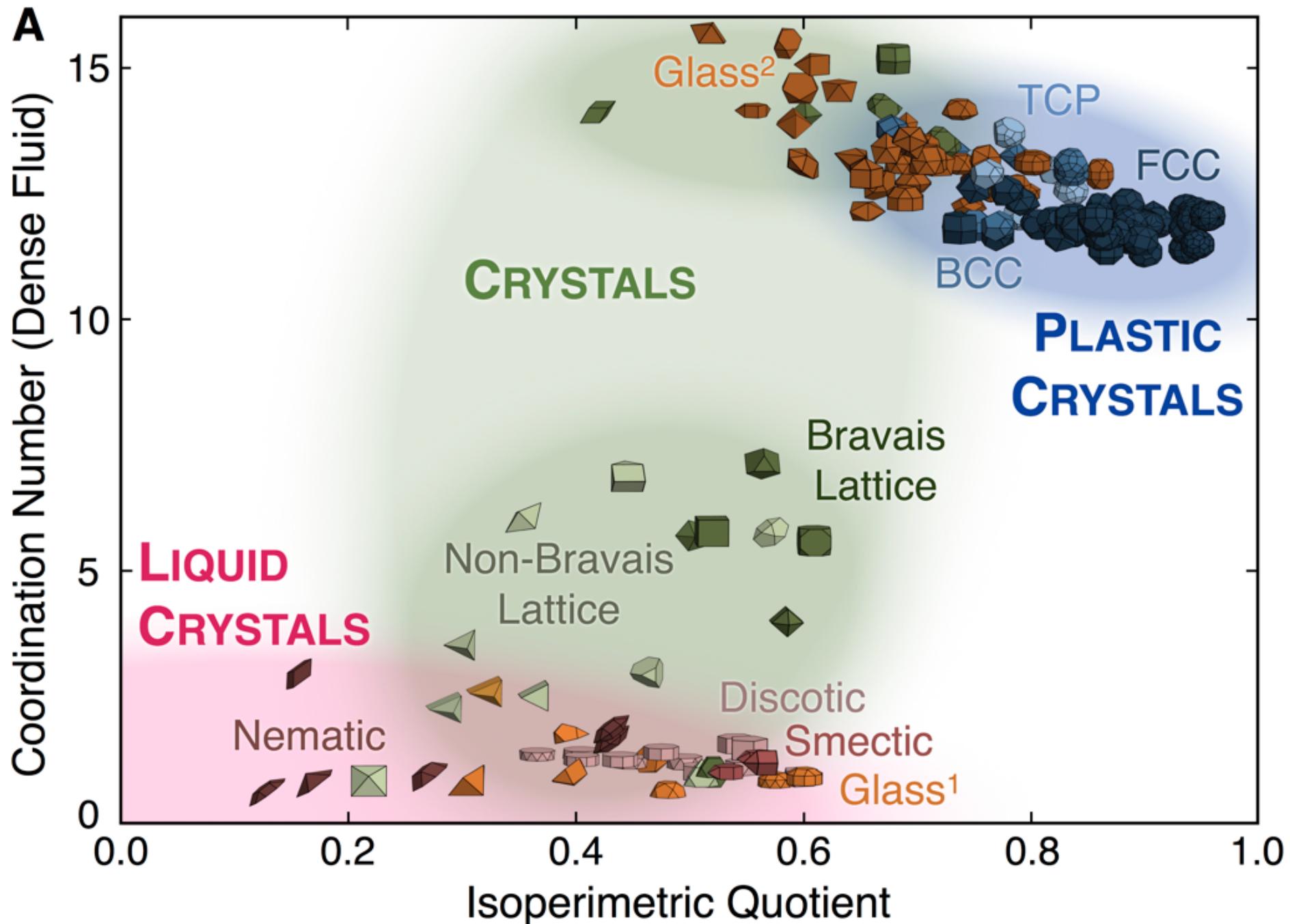






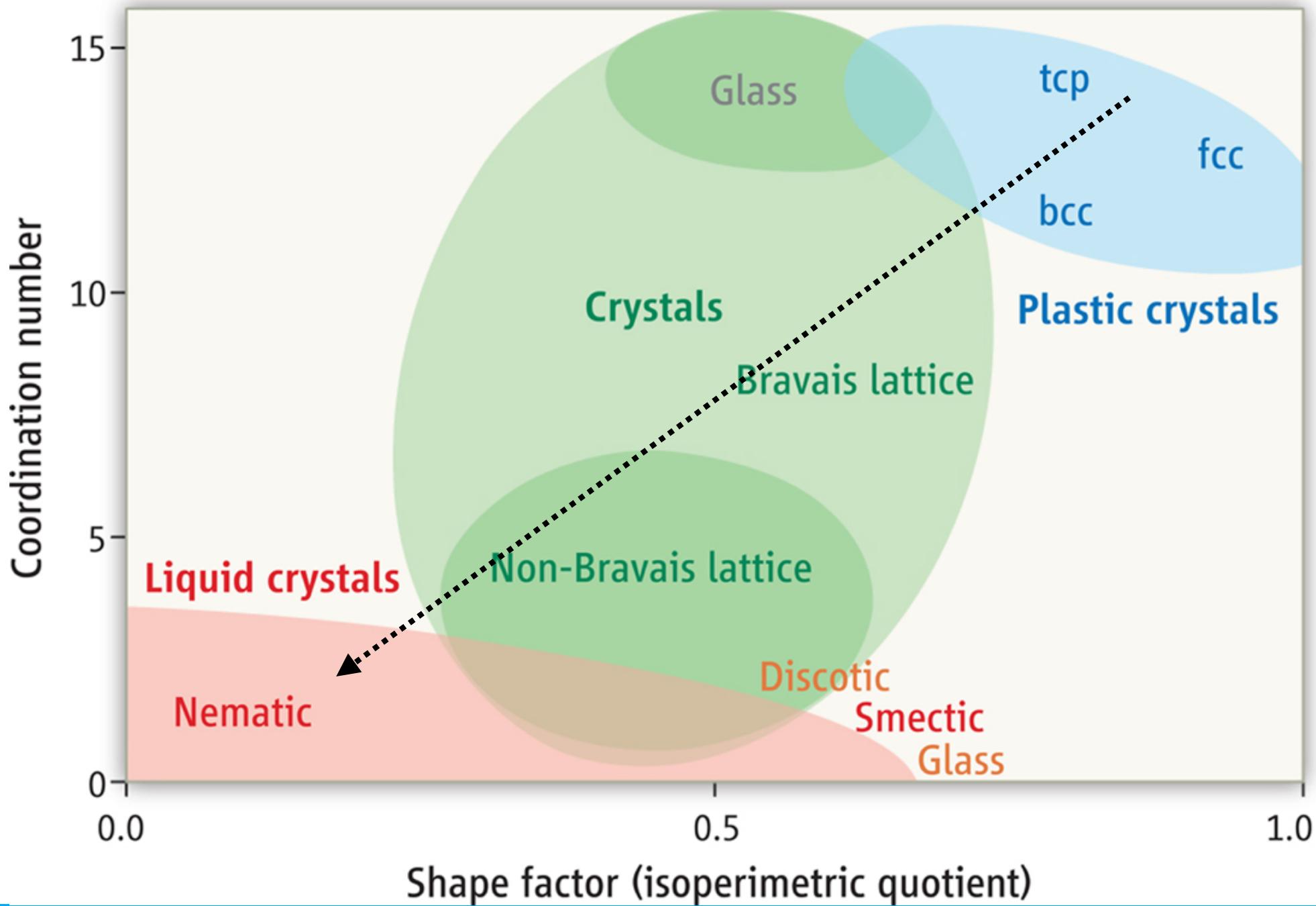


Predictable Assembly:

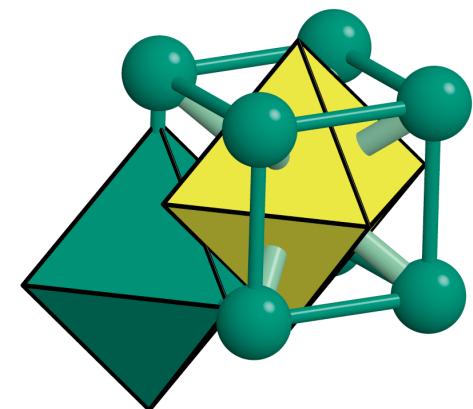
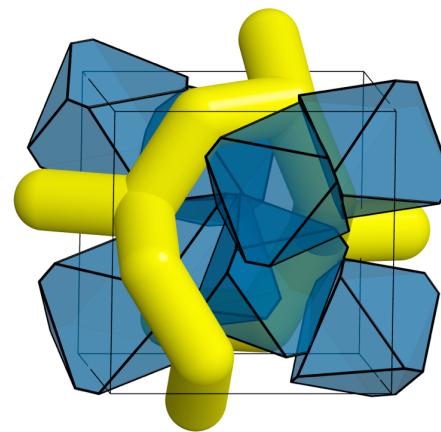
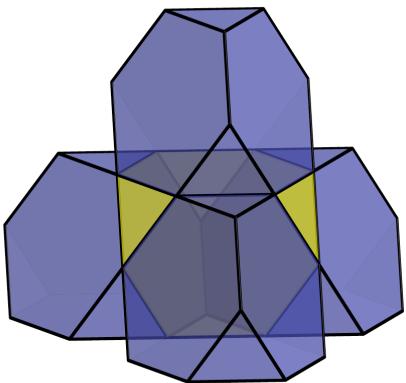
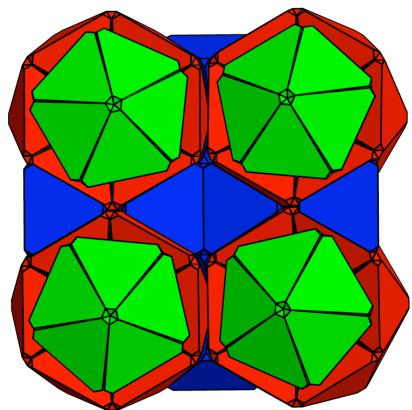


A Roadmap for the Assembly of Polyhedral Particles

Joost de Graaf, Liberato Manna
SCIENCE PERSPECTIVE (2012)



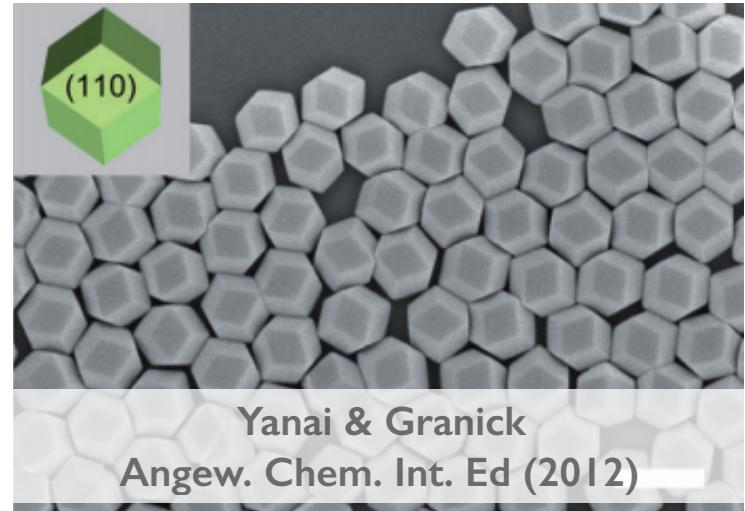
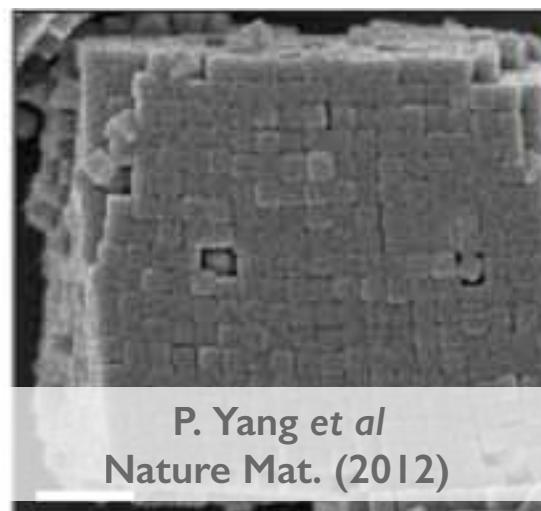
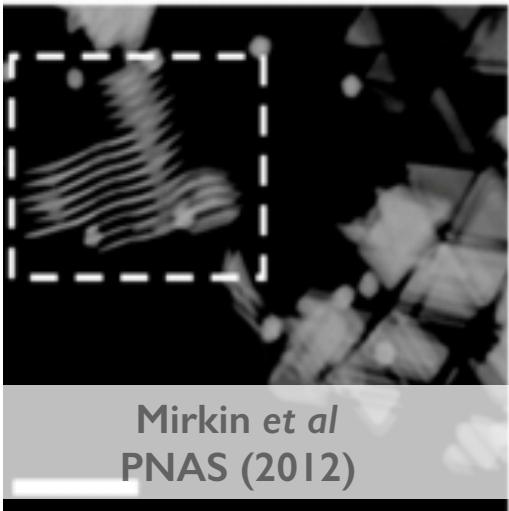
Entropic forces lead to assembly



Directional
Entropic Forces



Facetted particles tend to align their faces with maximum registry to maximize entropy

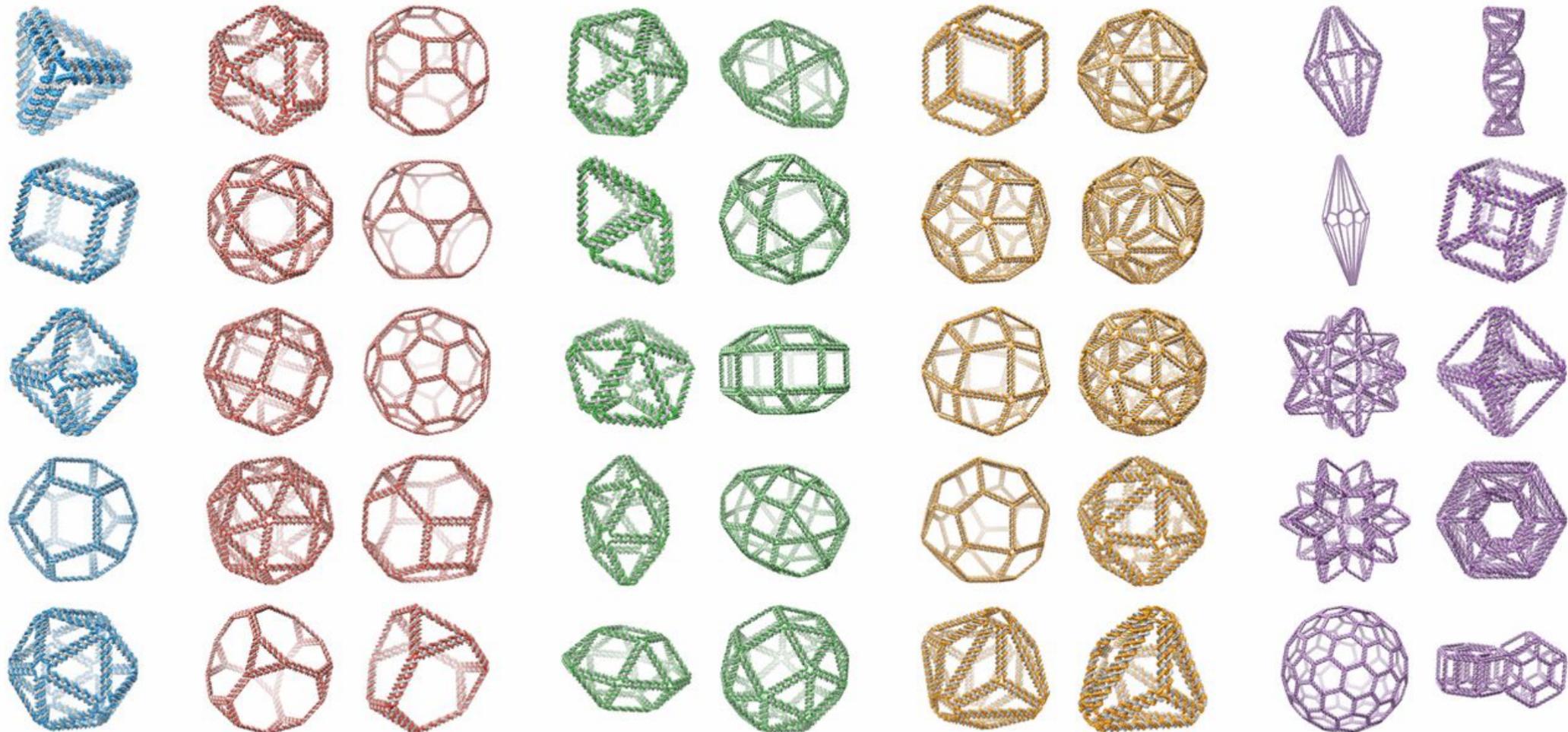


How about...



DNA ?

How about... DNA ?



Platonic

Archimedean

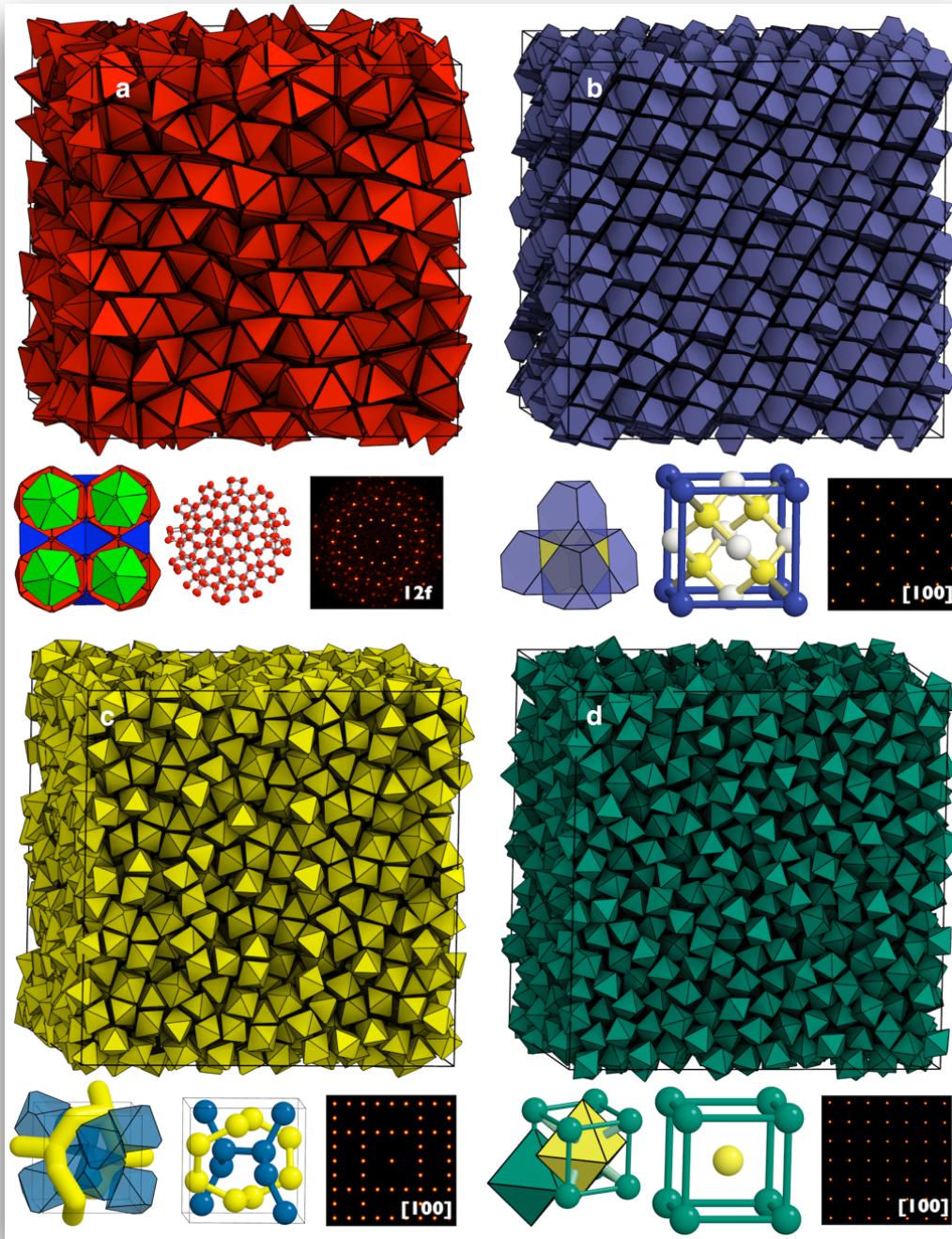
Johnson

Catalan

Miscellaneous

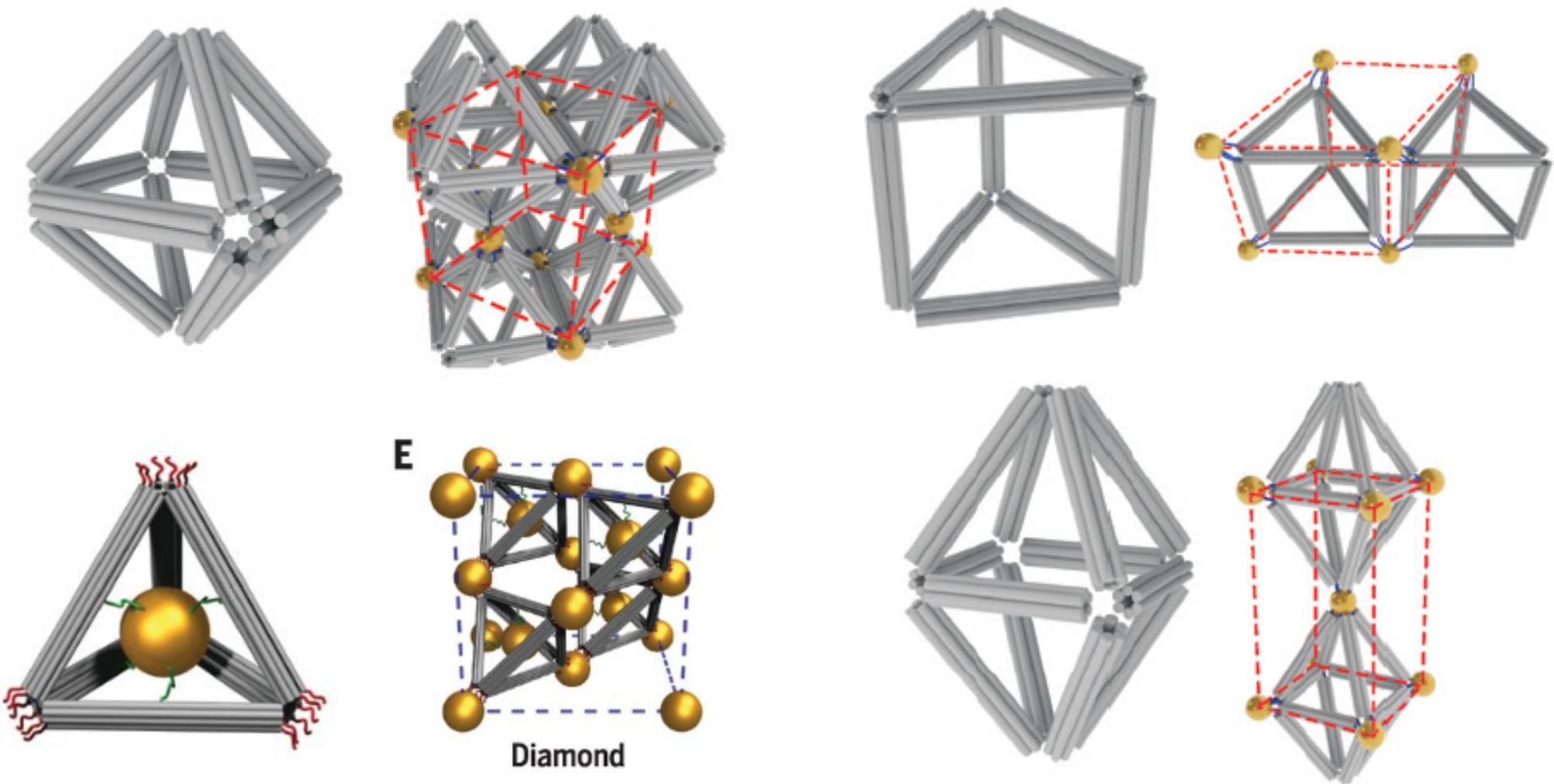
How about... DNA ?

?



?

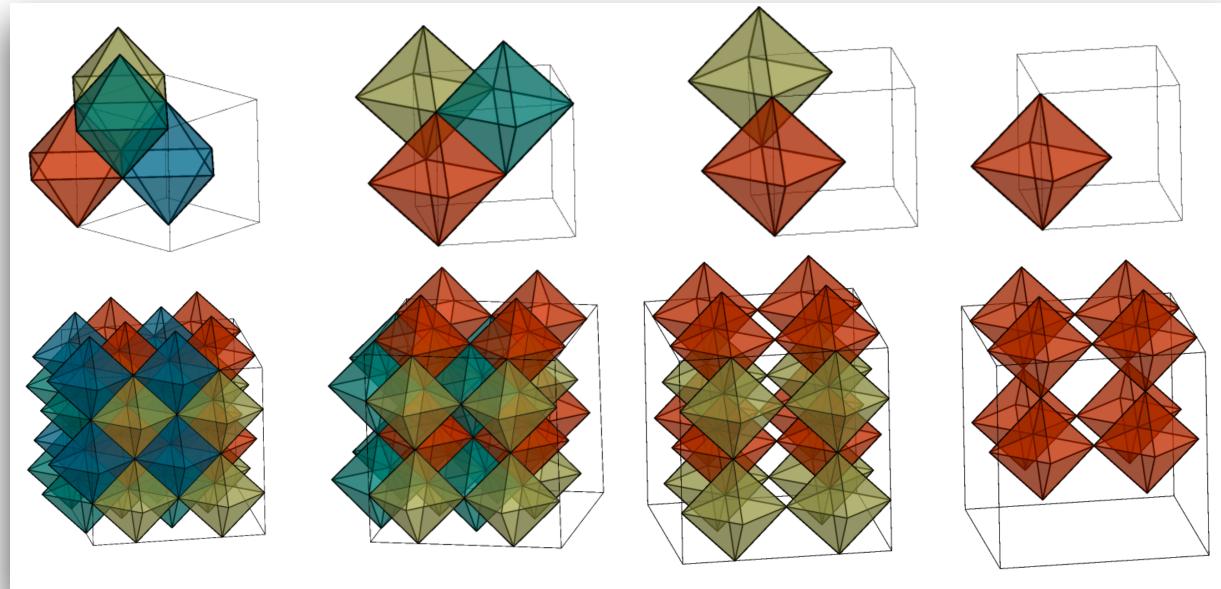
Crystal lattices achieved from DNA polyhedra and NPs



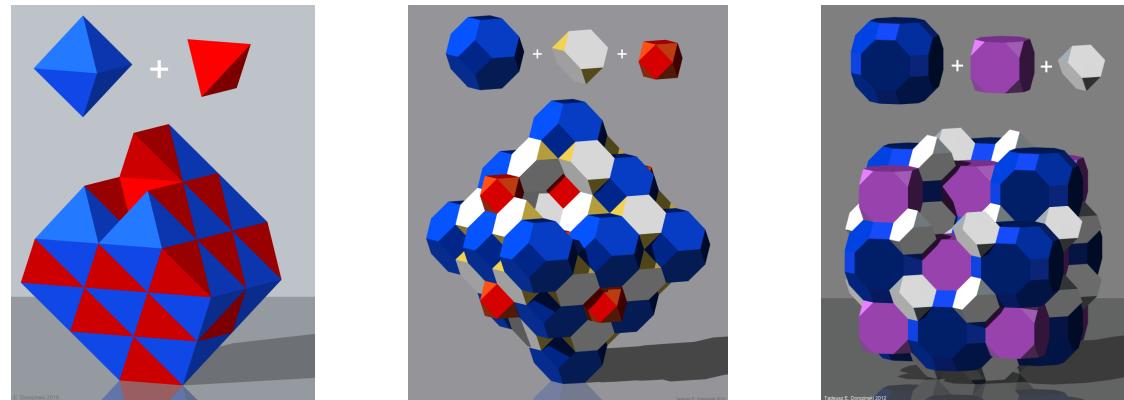
Gang et al.
Science (2015)
Nature Materials (2016)
Nature Chemistry (2016)

Open questions:

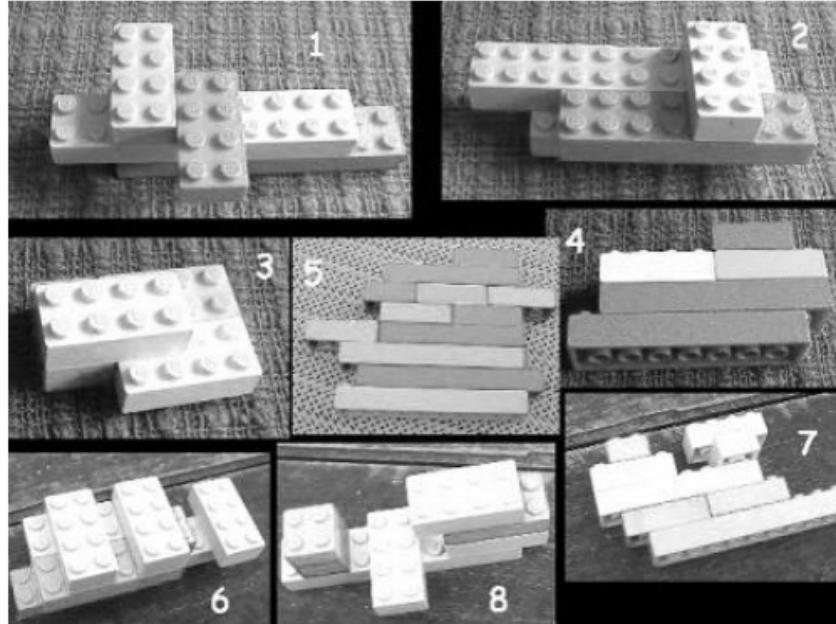
1. What dictates the assembly formation?



2. What about other shapes?



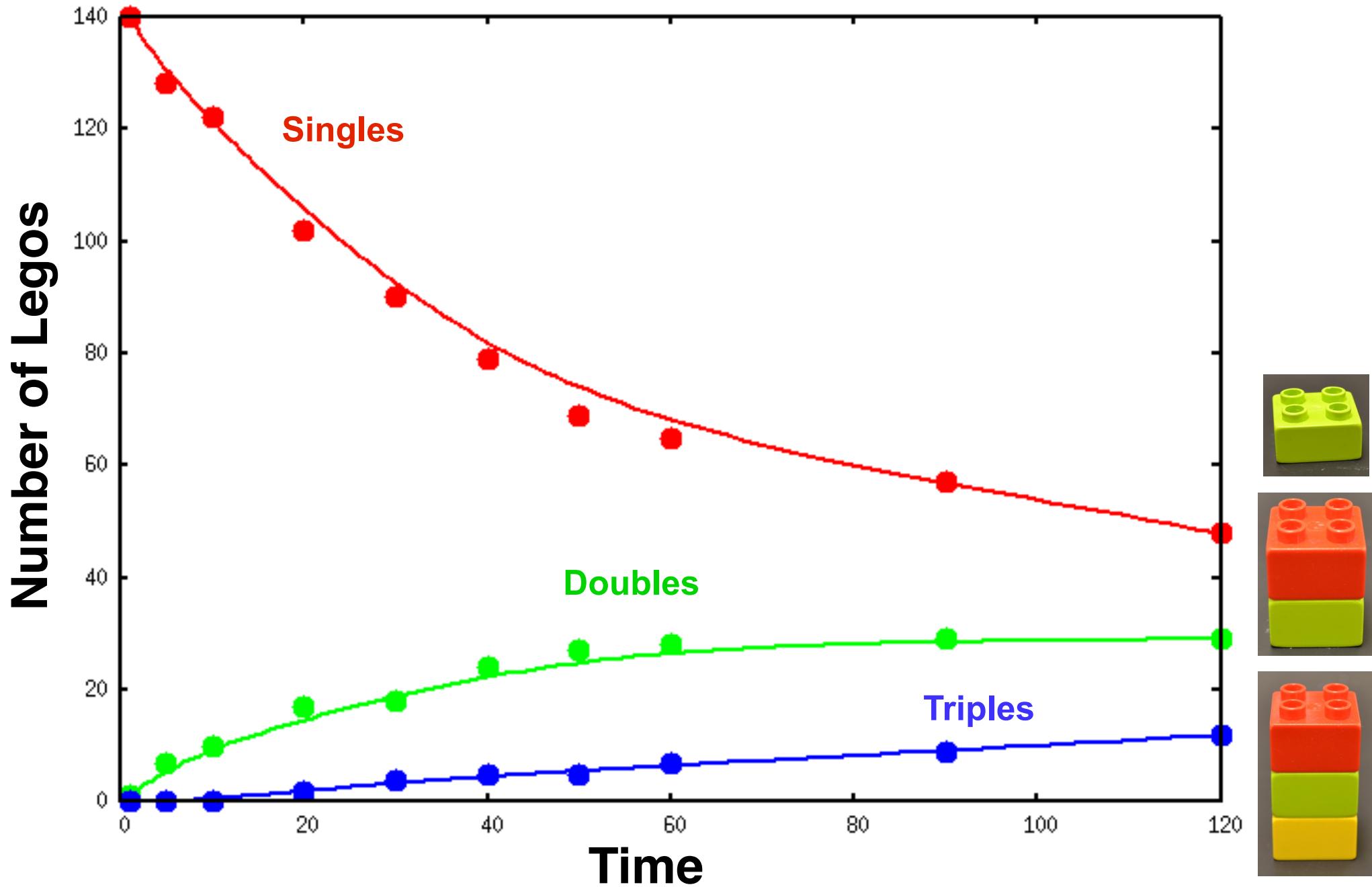
Lego: A Toy Model for Self-Assembly ?



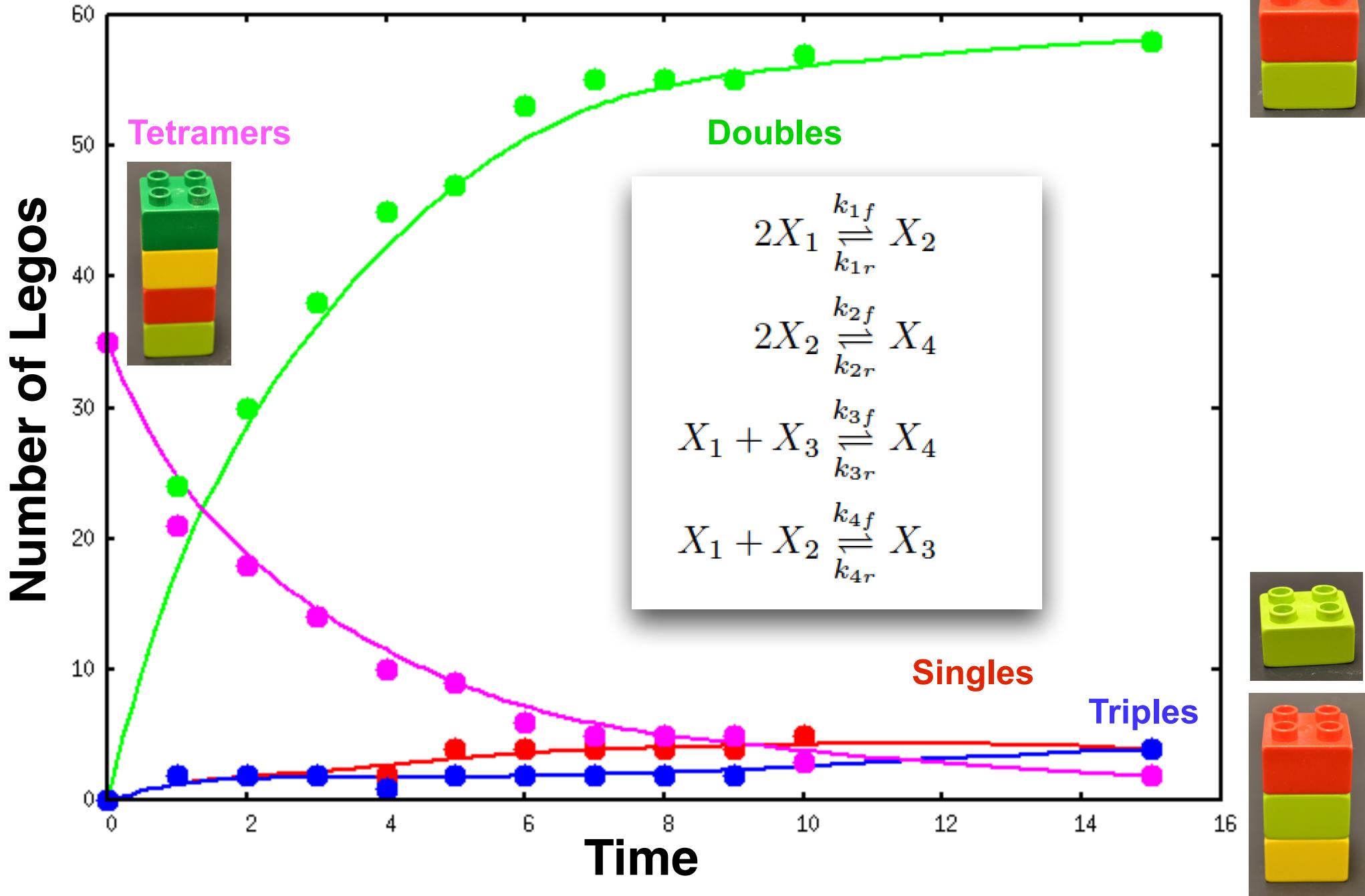
ps: heater off, please!

www.gizmodo.com

“Complex” Structure Formation



“More Complex” Structure Decay



Conclusions

- Self-Assembly allows the crystallization of very complex crystals from simple building blocks
- Entropy can lead to the assembly of *ordered* structures
- Shape + entropy can lead to *predictable complex crystal assemblies*
- The assembly principles governing DNA-origami polyhedra remain unknown

Thank you.

