Molecular Self-assembly (of proteins)

Introduction to Biophysics: Class 1

Definition: spontaneous association of small building blocks (atoms, molecules, or proteins) into large, stable structures using non-covalent bonds

(Seto, CT and Whitesides, GM, 1992)

Hydrogen bonds
Van der waal interactions
Hydrophobic interactions
Charge-charge interactions

"Molecular self-assembly is ubiquitous in nature and has recently emerged as a new approach in chemical synthesis, nanotechnology, polymer science, materials and engineering"

(Shuguang Zhang, MIT)

Self-assembly in Cells

- DNA single strands anneal by hydrogen bonds
- Proteins folding is guided by hydrogen bonds, Van der Waal interactions, hydrophobic interactions, etc.
- Lipids assemble into micelles due to hydrophobic interactions

Important Non-covalent interactions

- Hydrogen bonding: attraction b/w hydrogen bound to an electronegative atom and an electronegative atom bound to another atom
- Hydrophobic interactions
- Charge-charge interactions
- Van der Waals

Can anyone name the non-covalent interactions?

Which is the weakest non-covalent interaction?

A. hydrogen bonding in water
B. hydrogen bonding in DNA
C. charge-charge interactions
D. van der Waals forces

Collagen is the most abundant protein in our bodies. It makes up ~30% of the total protein.

A small collagen fibril consists of 3 peptides twisted into a helix. As the strands assemble in the water solvent, the "water-fearing" amino acids face the inside, while the polar amino acids face the water solvent. What non-covalent forces are involved in the folding of the protein?

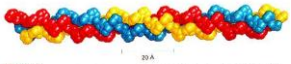
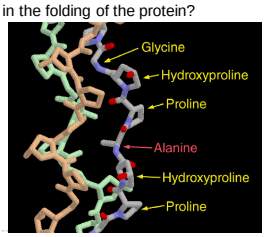
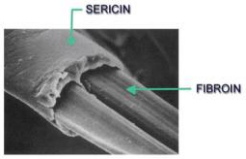


Figure 2-40
Space-filling model of the collagen triple helix. The three strands are shown in different colors. (Drawn from coordinates reported in K. Okuyama, K. Okuyama, S. Arnott, M. Takayanagi, and M. Kakudo, *J. Mol. Biol.* 152(1981):427.)

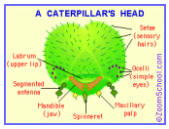


Silkworm's Silk: Self-assembly in Nature

- Consists of a core fiber (fibroid) wrapped around a sticky protein coat (sericin)



Silkworm's silk



- Fibroin exists a gel stored in gland of the silkworm. As it is extruded from a duct (spinneret), it becomes a stiff, insoluble fiber.

(Jin, HJ and Kaplan, D., 2003 Nature)

Spider's Silk

- 10x stronger than steel
- stretches 40% more than normal length
- Bulletproof vest (stronger than kevlar), bandages, airbags
- History: Madagascar textile (11'x4', 2.6 lbs)

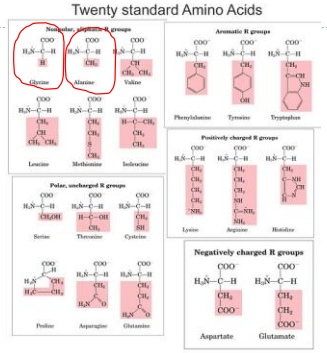
http://www.wired.com/wiredscience/2009/09/spider-silk/

Genetically engineered silkworm silk

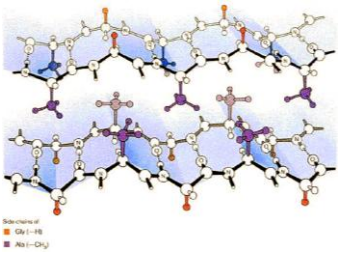
- University of Notre Dame & Biocraft Labs

http://newsinfo.nd.edu/news/16934-notre-dame-and-university-of-wyoming-scientists-genetically-engineer-silkworms-to-produce-artificial-spider-silk/?utm_source=feedburner&utm_medium=feed&utm_campaign=Feed%3A+NewsAndInformation%2FResearch+(News+and+Information+-

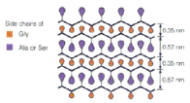
Twenty standard Amino Acids



Fibroin structure

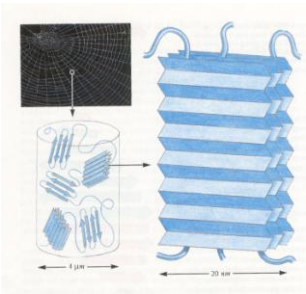


- 80% beta sheet
- Alternating glycine and alanine amino acids



http://www.biostat.jhsph.edu/~iruczins/teaching/260.655/notes/prjpge2.3.pdf

Beta Pleated sheets of Fibroin



http://www.uic.edu/classes/phys/phys461/phys450/ANJUM05/

Advantages of Self-Assembly

In contrast to polymers made from petrochemicals:

- Can occur at room temperature (chemical processes require higher temperature)
- Can produce with less energy input
- Less toxic starting materials (use water instead of harsh solvents)

(Vollrath, F. and Knight, DP, 2001, Liquid crystalline spinning of spider silk)

Micropottery

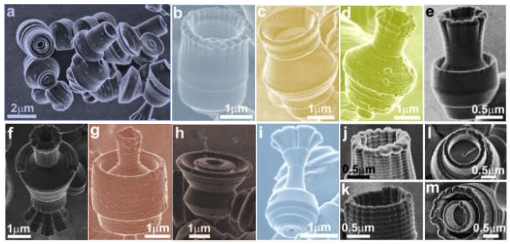
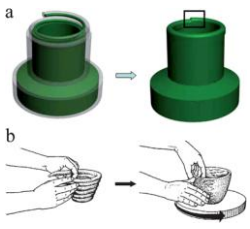
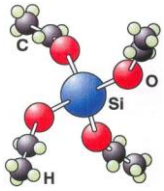


Fig. 1 SEM images of mesostructured silica micropottery vessels.

Micropottery: TEOS





http://www.oxfordplasma.de/process/sio_teo
m

(Zhou, L, et. al, 2011)

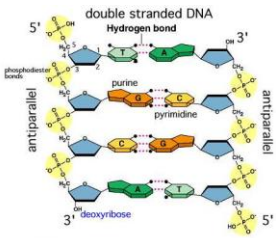
Scheme 1 (a) Schematic illustration of spontaneous coiling of mesostructured silica nanofibers into micropottery vessels. The boxed area indicates the presence of a breakpoint on the vessel rim. (b) Manufacture of pottery vessels by wheel shaping in Oriental Asia during the 4th to 3rd millennium BC. Reprinted with permission from ref. 17, copyright 1998 Academic Press.

Case 1: DNA origami

- http://en.wikipedia.org/wiki/DNA_origami
- http://news.bbc.co.uk/2/hi/technology/8204906.stm
- What are the applications?
- How are the patterns formed?

http://en.wikipedia.org/wiki/DNA_origami
http://news.bbc.co.uk/2/hi/technology/8204906.stm

DNA Hydrogen Bonds



Chemical Bond Strengths

Bond type	Energy (kJ/mol)
Covalent, e.g. C-C	350
Electrostatic	15
Van der Waal's	10
Hydrogen	21

http://www.ncbi.nlm.nih.gov/books/NBK21726/