భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్
भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

Biomolecular Simulation BT2123

Lecture 5 : Creating an all-atom model of DNA

Himanshu Joshi 30 January 2024

Course contents

- Historical perspective
- Foundations of Molecular Mechanics (MM)
- **Statistical ensembles**
- Quantum Mechanics (QM)
- Introduction molecular dynamics simulations
- Equation of motion,
- Force-fields, Scheme of integrations,
- Langevin Dynamics,
- Non-bonded Computations,
- Brownian Dynamics,
- Monte Carlo Techniques,
- Coarse Graining Models

Reading material

Who discovered DNA ?

https://www.nature.com/scitable/topicpage/discovery-of-dna-structure-and-function-watson-397/

Friedrich Miescher, 1869

doi:10.1006/jmbi.2001.4987 available online at http://www.idealibrary.com on IDEAL® J. Mol. Biol. (2001) **313**, 229–237

JMB

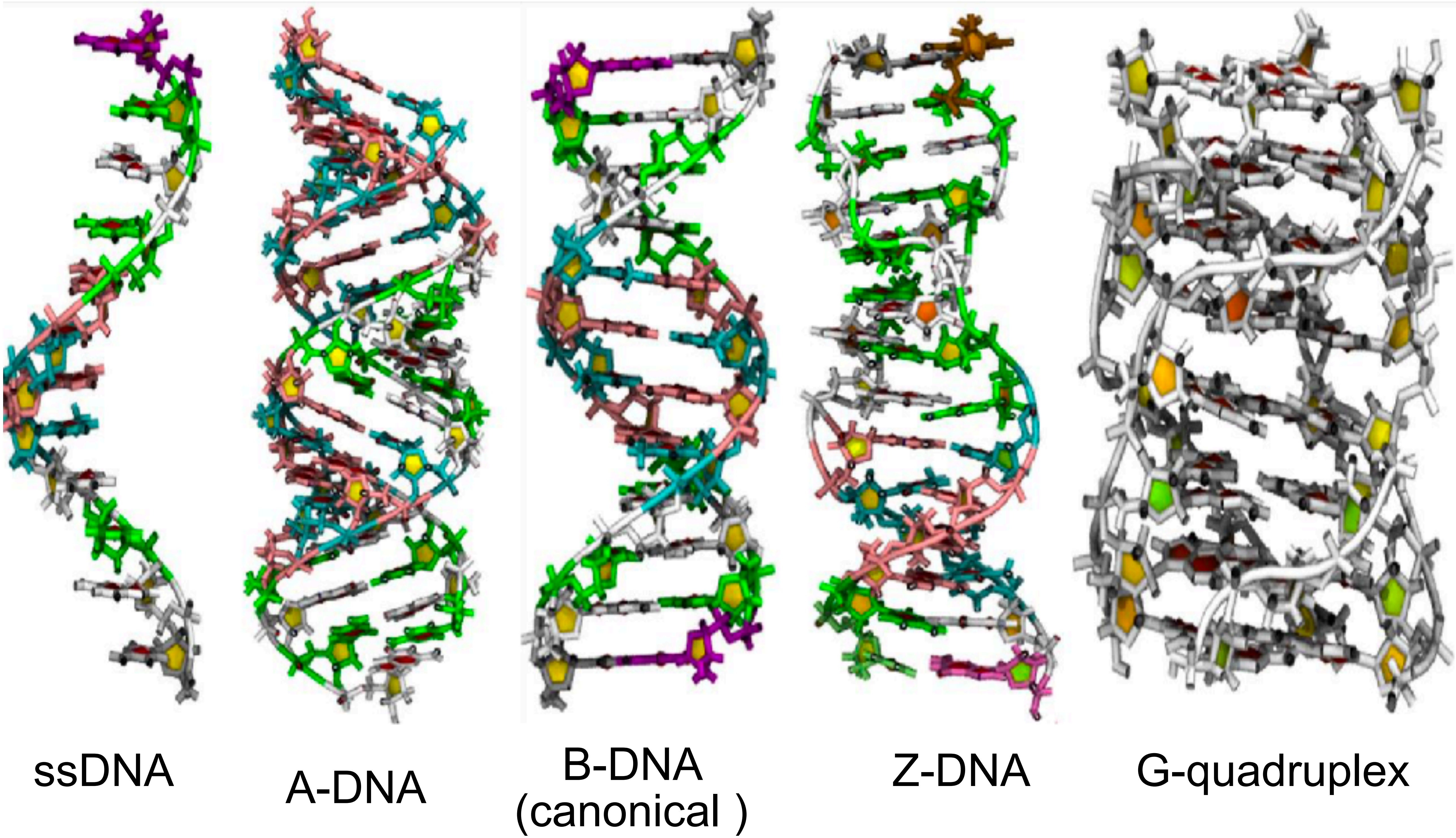
NOMENCLATURE

A Standard Reference Frame for the Description of Nucleic Acid Base-pair Geometry

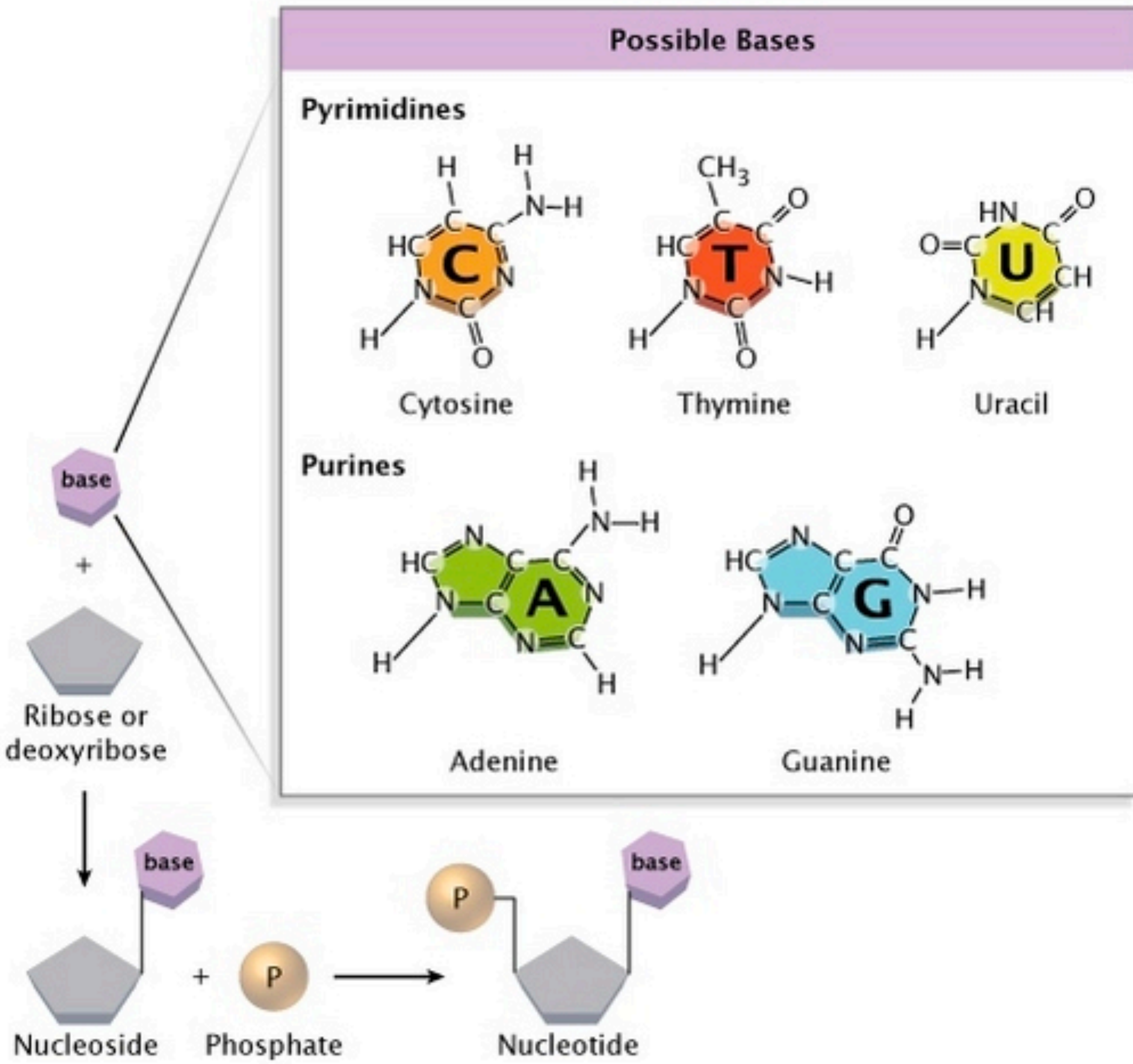
Wilma K. Olson, Manju Bansal, Stephen K. Burley
Richard E. Dickerson, Mark Gerstein, Stephen C. Harvey
Udo Heinemann, Xiang-Jun Lu, Stephen Neidle, Zippora Shakked
Heinz Sklenar, Masashi Suzuki, Chang-Shung Tung, Eric Westhof
Cynthia Wolberger and Helen M. Berman

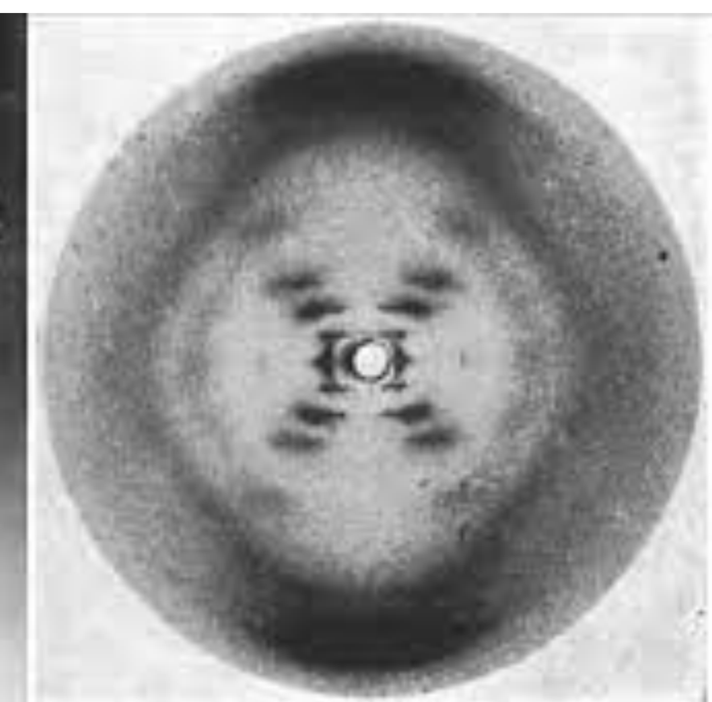
Keywords: nucleic acid conformation; base-pair geometry; standard reference frame

Various forms of DNA



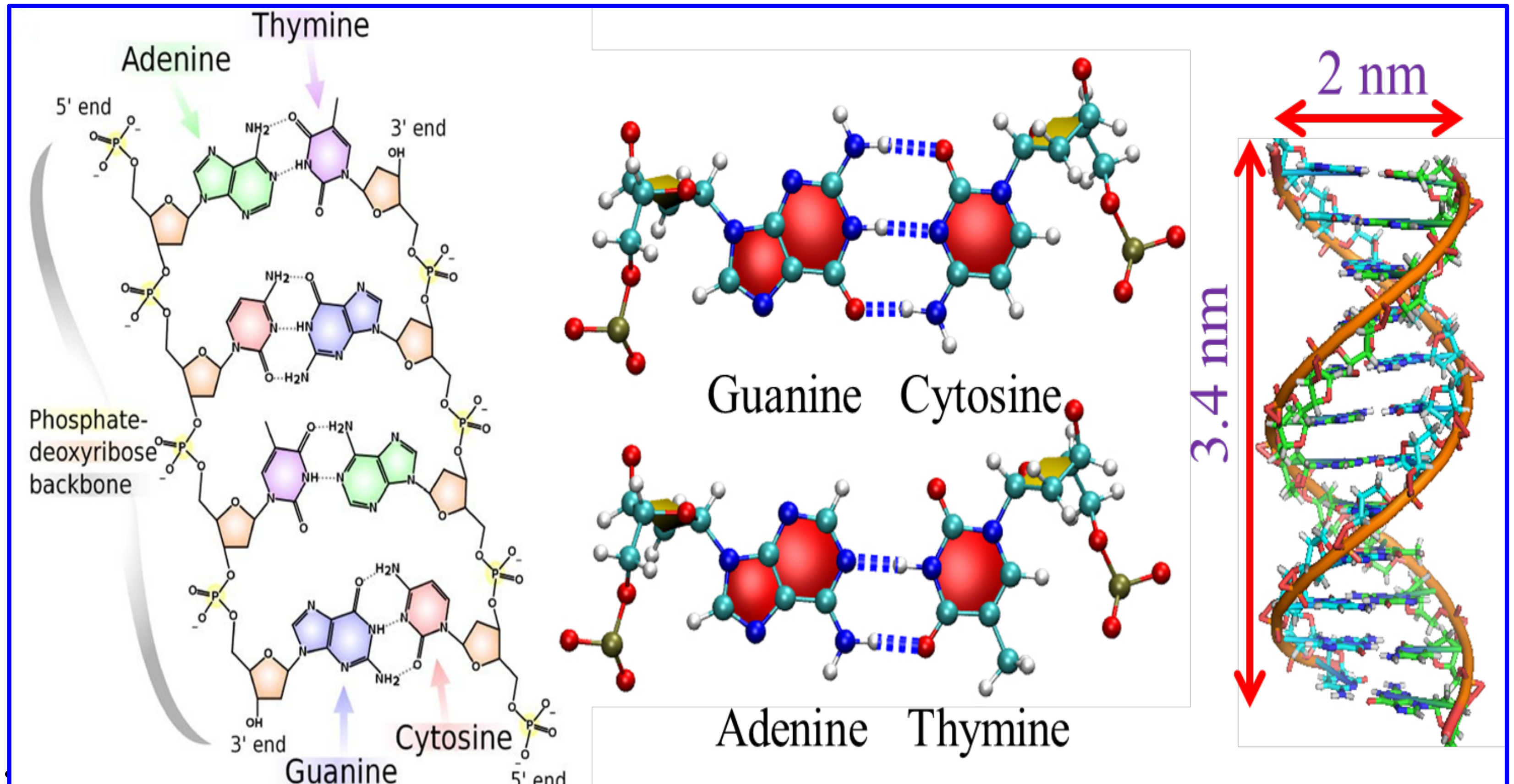
3 D structure of DNA



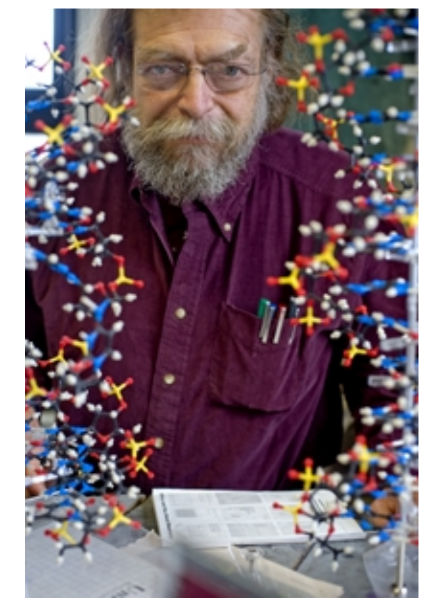


Structural DNA Nanotechnology

- There is plenty of room at the bottom.
- Bottom up self-assembly : DNA as a construction material



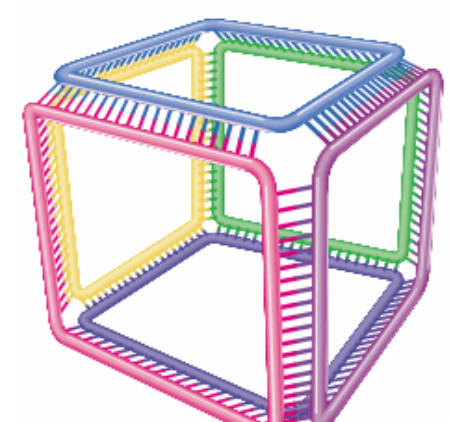
R. Feynman



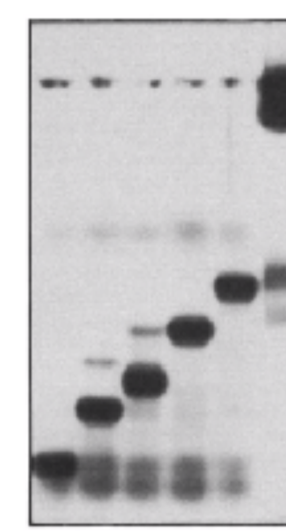
N. Seeman

Why DNA

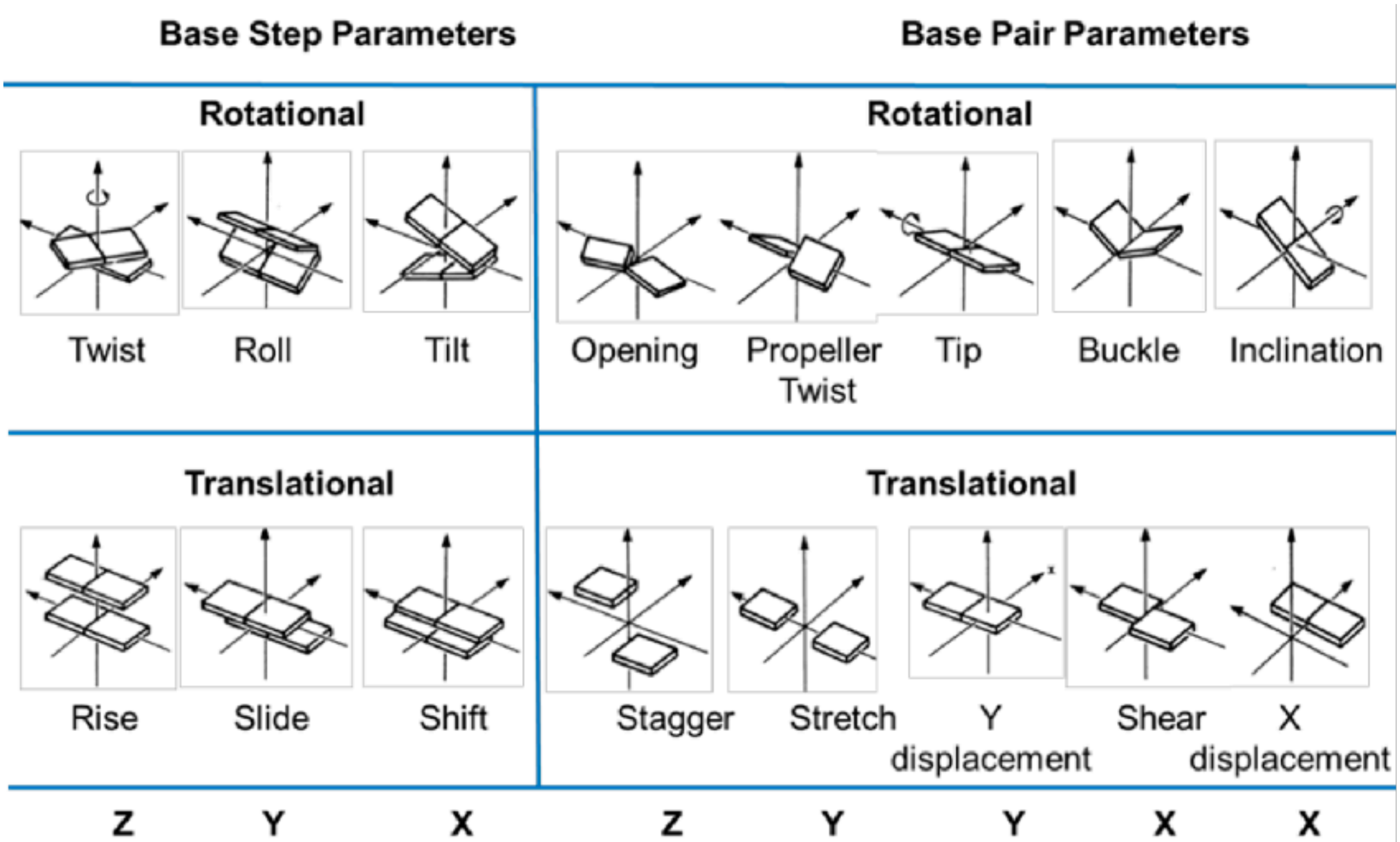
1. Molecular recognition property
2. Chemically easy to modify the backbone
3. Well studied molecule.



DNA cube, Chen and Seeman. Nature 1991



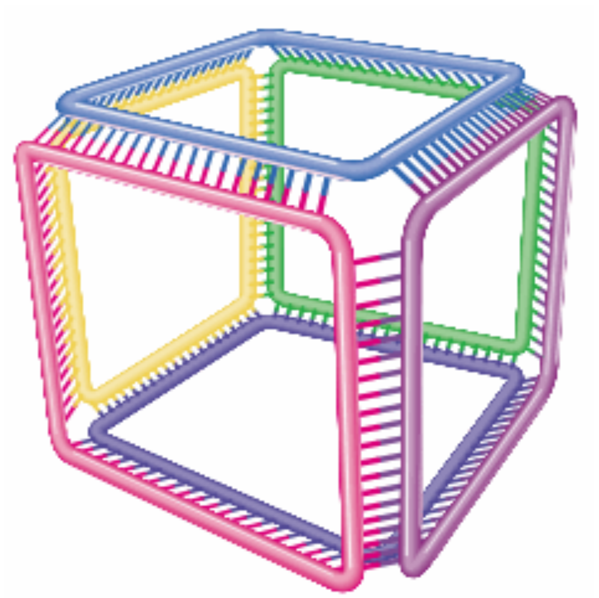
Geometrical parameters characterizing the structure of dsDNA



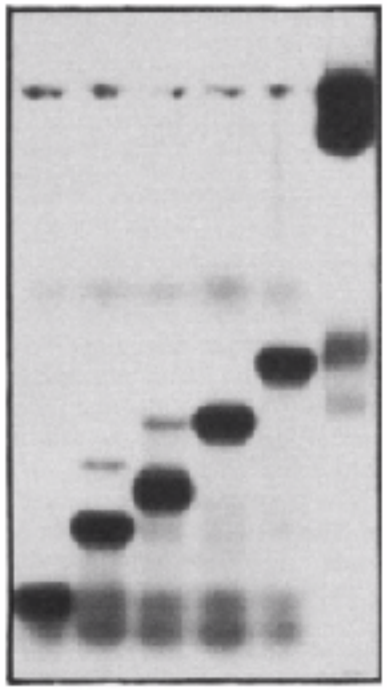
Geometrical parameters of various form of dsDNA

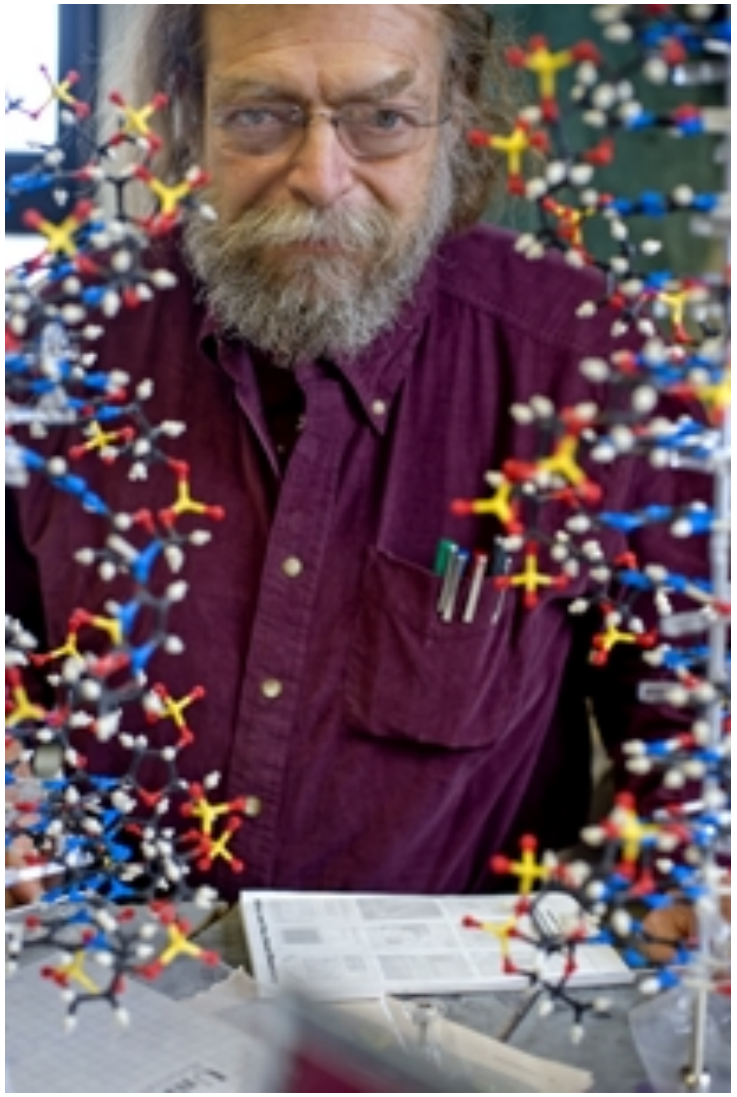
Structure	Helical Twist	Helical Rise	X-Displ	Inclin.	Roll	Propeller Twist	Diameter
A-DNA	33°	2.56 Å	-4.5 Å	21°	6°	-7.5°	23 Å
B-DNA	36°	3.38 Å	0.23 Å	-6°	0°	-4.4°	20 Å
Z-DNA	-30°	3.7Å	3.0 Å	-6.2°	0°	-4.4°	18 Å

DNA Nanotechnology



DNA cube,
Chen and Seeman. Nature 1991





DNA Nanotechnology

- A method to create nanoscale object using DNA/RNA as construction material
- Incepted by Nadrian C. Seeman, in 1982 to crystalize protein which is a very hard problem to solve.
- The field was inspired by using DNA nanostructure as a tool to in biophysics but now taken as a entire

Chemist saw it as a water-soluble polymer whose growth could be controlled and whose branching, or cross-linking, could be rationally manipulated.

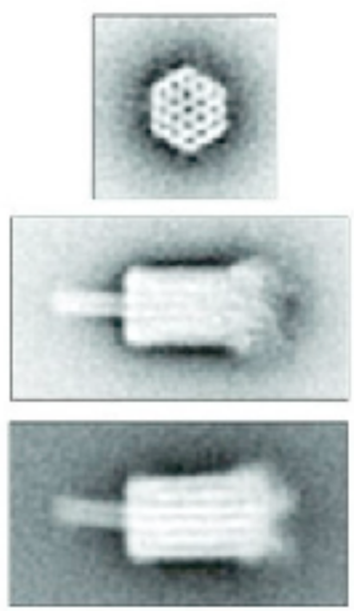
Yamuna and Ned, 2019

Ned Seeman
1945-2021

DNA Origami

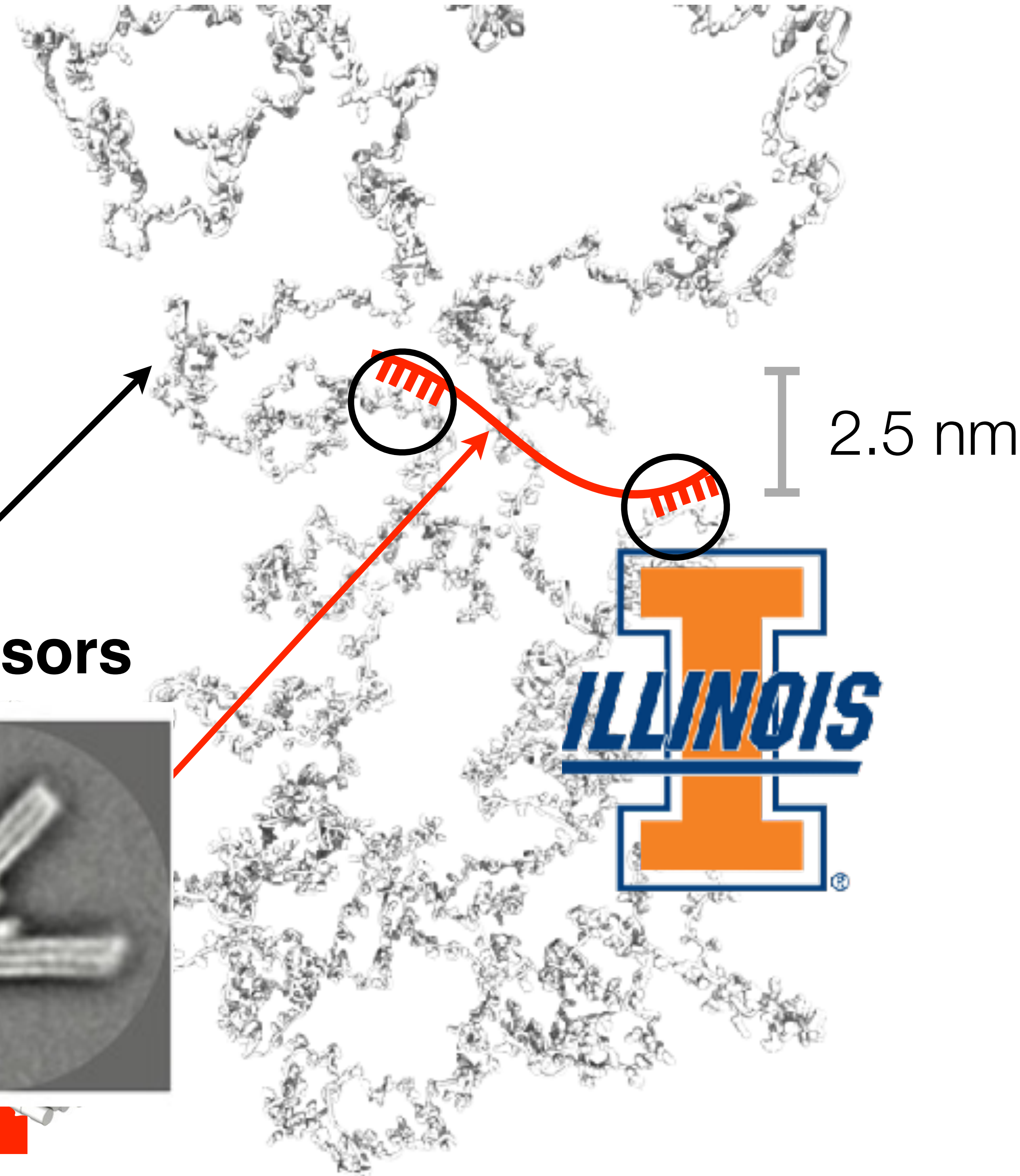
Custom shapes, channels, and sensors

Nature 2005
Paul Rothemund



Science 2012
Simmel el al.

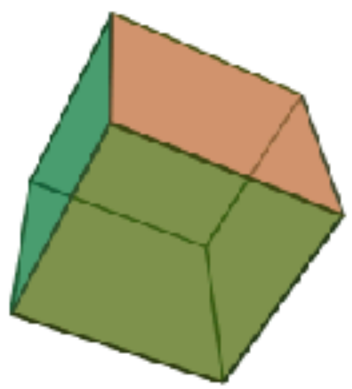
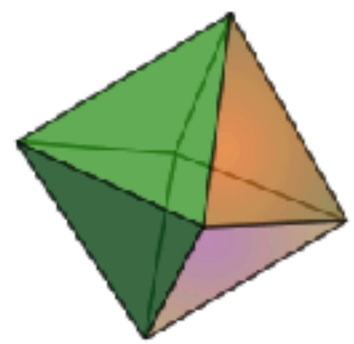
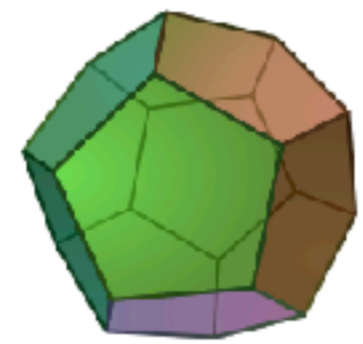
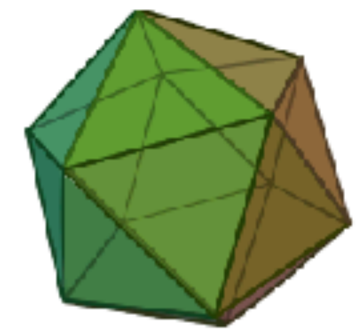
Science Adv. 2016
Dietz et al.



Source: J. Yoo, Aksimentiev lab

Platonic solids

Only five convex regular polyhedron exist in 3d euclidian space

Tetrahedron	Cube	Octahedron	Dodecahedron	Icosahedron
Four faces	Six faces	Eight faces	Twelve faces	Twenty faces
				

Parameters

Figure	Tetrahedron		Octahedron	Cube	Icosahedron		Dodecahedron	
Faces	4		8	6	20		12	
Vertices	4		6 (2 × 3)	8	12 (4 × 3)		20 (8 + 4 × 3)	
Position	1	2			1	2	1	2
Vertex coordinates	(1, 1, 1) (1, −1, −1) (−1, 1, −1) (−1, −1, 1)	(−1, −1, −1) (−1, 1, 1) (1, −1, 1) (1, 1, −1)	(±1, 0, 0) (0, ±1, 0) (0, 0, ±1)	(±1, ±1, ±1)	(0, ±1, ±ϕ) (±1, ±ϕ, 0) (±ϕ, 0, ±1)	(0, ±ϕ, (±ϕ, ±1, (±1, 0, ±ϕ)	(±$\frac{1}{\phi}$, ±ϕ, 0) (±ϕ, 0, ±$\frac{1}{\phi}$)	(±ϕ, ±$\frac{1}{\phi}$, 0) (±$\frac{1}{\phi}$, 0, ±ϕ)

Virus assembly

Using VMD

Download VMD

https://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node1.html

Visualizing a cube in VMD

Tcl programming

Usage: Visualization, Building models, Analysis of simulation Trajectories

Homework

Laws of thermodynamics

DNA translational and rotational parameters

Reading material