DNA Tiles & Lattices

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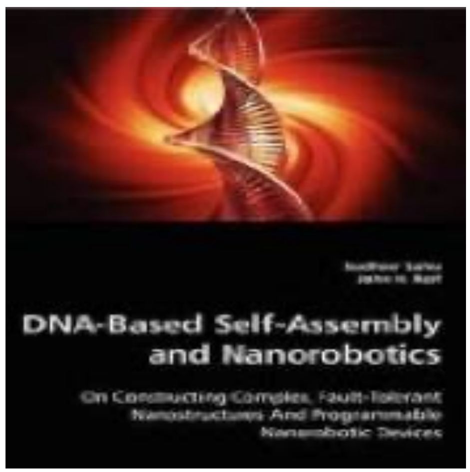

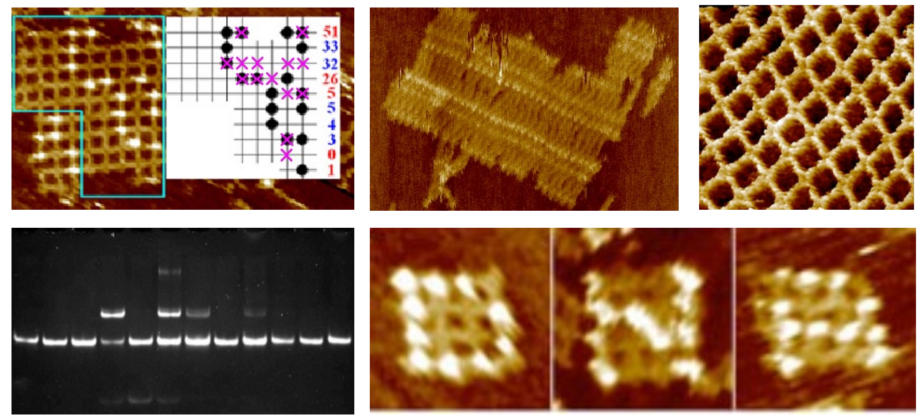

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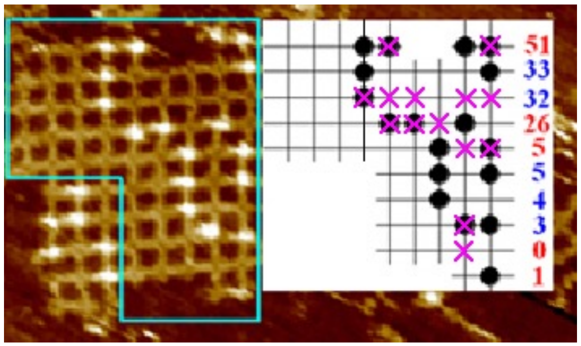

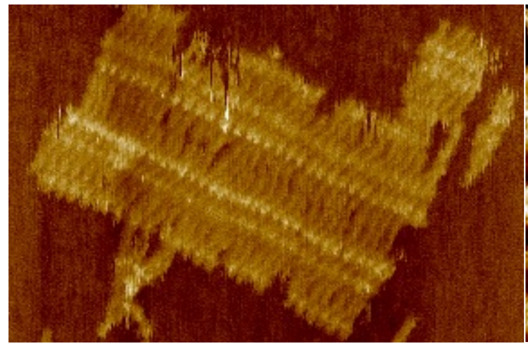

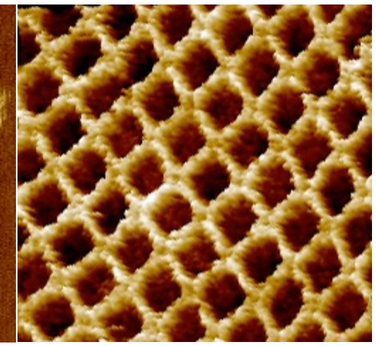

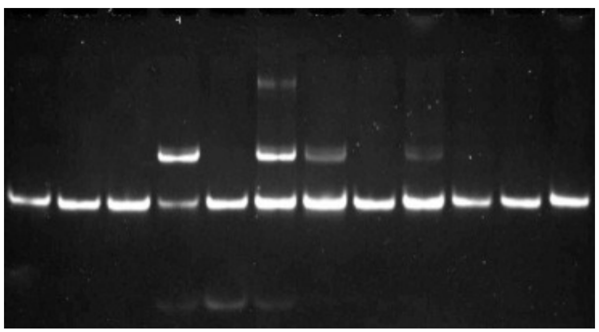

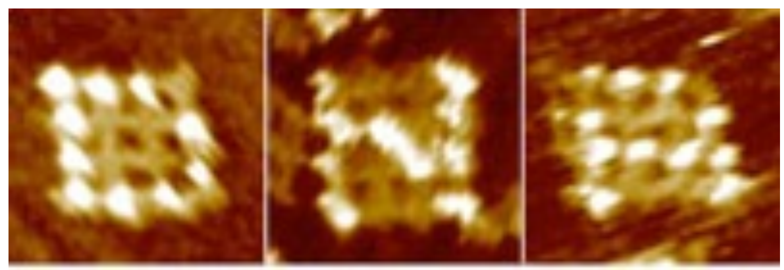

DUKE COMPUTER SCIENCE

Organization

- Overview of DNA & DNA Self-Assembly
- DNA Tiles
- 2D DNA Lattices
- Programmable Molecular Patterning via DNA Lattices
- Transformations of DNA Lattices
- 3D DNA lattices via double decker tiles

Introduction to DNA Self-Assembly

Feynman's Ill-Conceived Top-Down Approach to Nanotechnology

Feynman ("Plenty of room at the bottom", 1959):

- Can the doctor be swallowed? (Albert Hibbs)
- Can we build tiny factories that can arrange atoms the way we want?
- Can we write the 24 volumes of the Encyclopedia Brittanica on the head of a pin?

"This fact - that enormous amounts of information can be carried in an exceedingly small space - is, of course, well known to the biologists, and resolves the mystery which existed before we understood all this clearly, of how it could be that, in the tiniest cell, all of the information for the organization of a complex creature such as ourselves can be stored. All this information---whether we have brown eyes, or whether we think at all, or that in the embryo the jawbone should first develop with a little hole in the side so that later a nerve can grow through it - all this information is contained in a very tiny fraction of the cell in the form of long-chain DNA molecules in which approximately 50 atoms are used for one bit of information about the cell."

Self-assembly in nature:

Spontaneous organization of components into stable superstructures due to local interactions

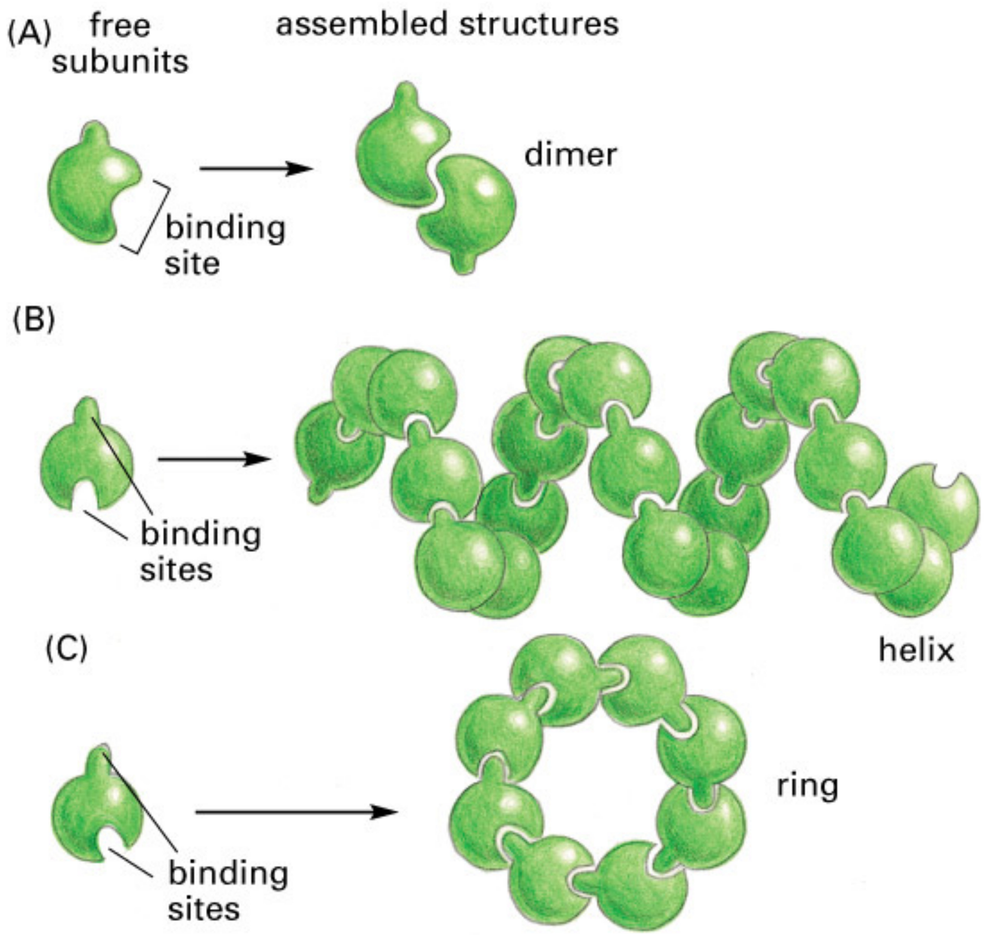

Figure 3–25. Molecular Biology of the Cell, 4th Edition.

From microscopic living cells to gigantic galaxies

Why study self-assembly?

- Brings about order from disorder.
    - Interesting at a philosophical level

- Plays a fundamental role in biology; in formation of living cell.
    - Attempt to understand life must include a through study of self-assembly.

- One of the few known methods for the construction and manipulation of nanostructures.

- Any Turing-computable function can be computed via self-assembly of Wang tiles:
    - New paradigm of computing
    - Lower bounds proved in theoretical self-assembled systems can be translated (by appropriate reductions) to Turing systems

Why use DNA for Self-Assembly of Nanostructures?

1. Natural nanoscale material
2. Ability to carry information can be exploited in self-assembly process
3. Well established base-pairing model in which the stability of a base-pair depends on their identity (A-T, C-G)

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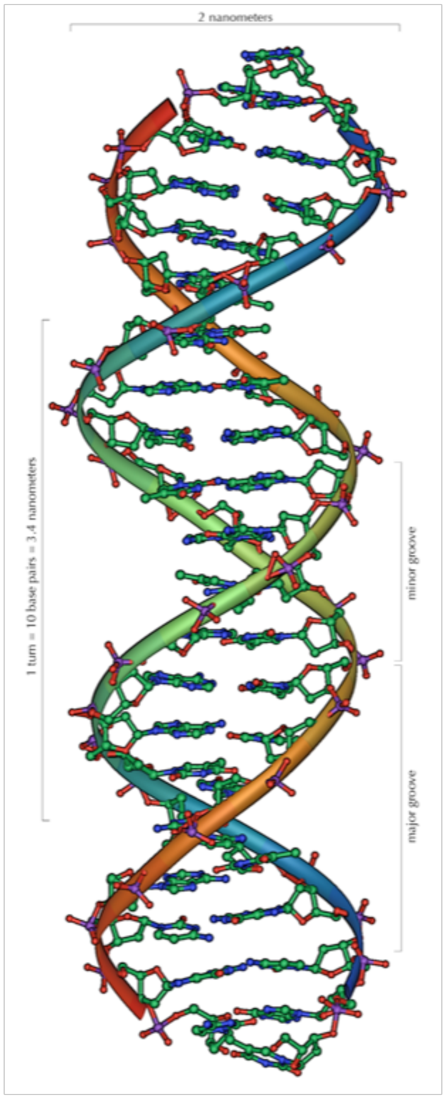
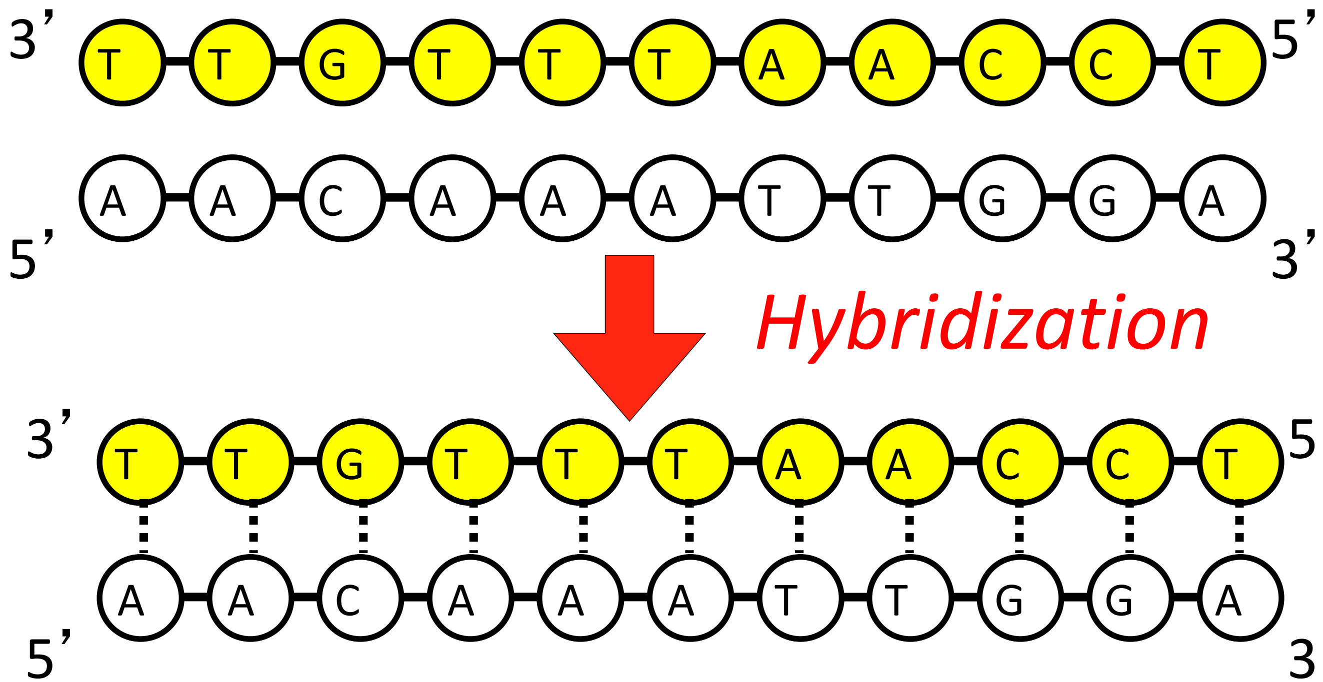
Key to DNA Self-Assembly





What is DNA Self-Assembly?

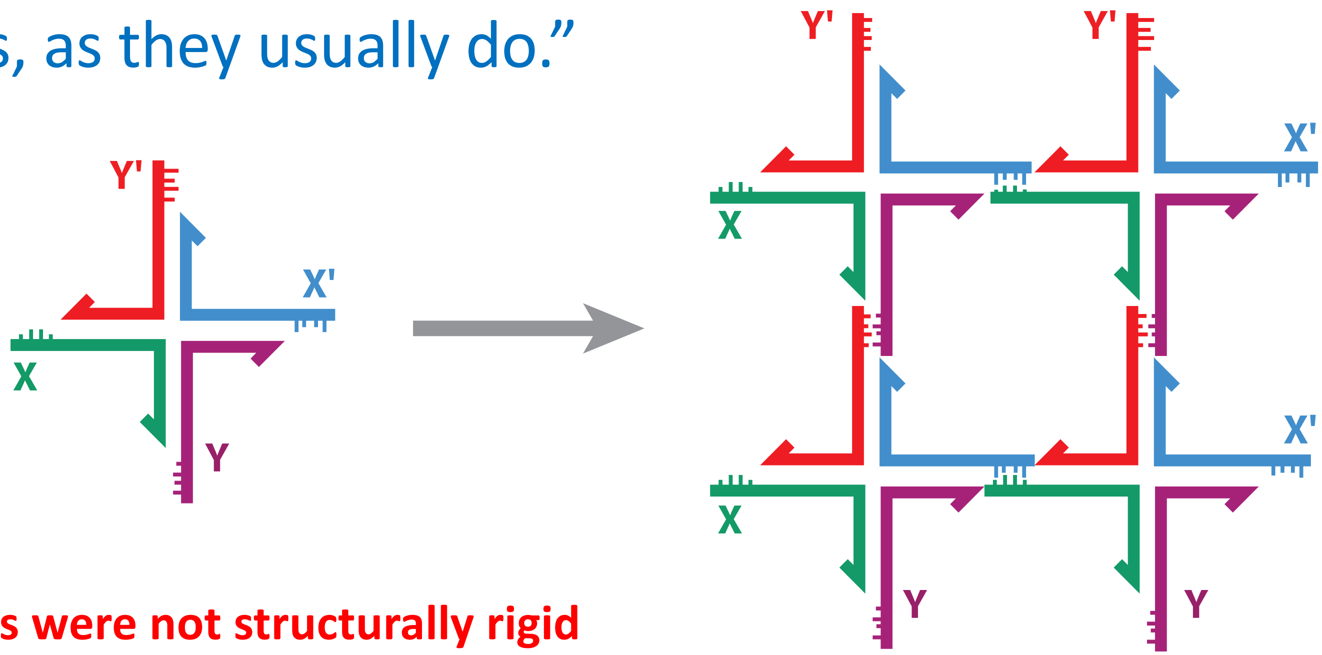
Programming DNA strands to organize themselves into nanoscale shapes, patterns, and devices through Watson-Crick base-pairing.

First Work in DNA Nanotechnology

Seeman 1982:

Seeman, N. C. (1982). Nucleic acid junctions and lattices. *Journal of Theoretical Biology*, *99*(2), 237–247. doi:10.1016/0022-5193(82)90002-9

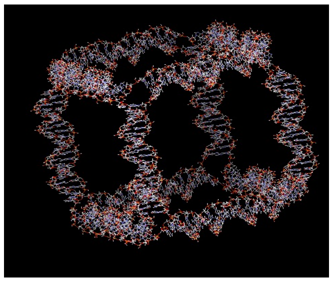
- "It is possible to generate sequences of oligomeric nucleic acids which will preferentially associate to form migrationally immobile junctions, rather than linear duplexes, as they usually do."



Note: These Tiles were not structurally rigid

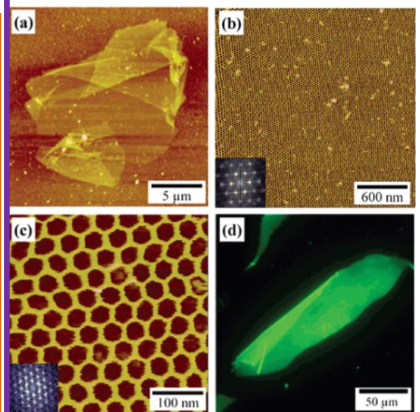
Some results of DNA self-assembly

NYU 1991



The Electrophoretic Properties Of A DNA Cube And Its Substructure Catenanes : Mao And Seeman

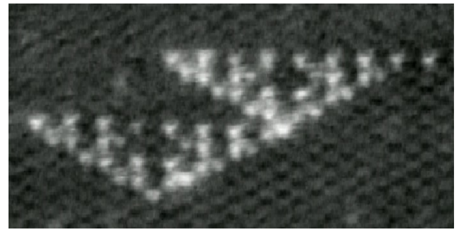
Purdue 2005



Self-assembly Of Hexagonal DNA Two-dimensional (2D) Arrays: He, Chen, Liu, Ribbe, And Mao

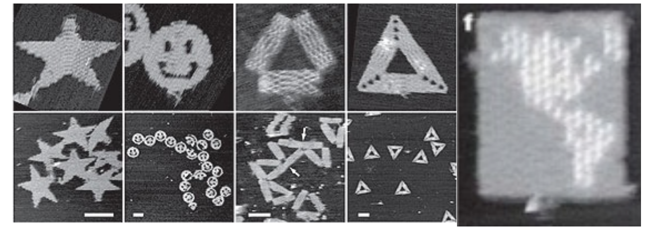
Caltech

2004



Algorithmic Self-assembly Of DNA Sierpinski Triangles: Rothemund, Papadakis, Winfree

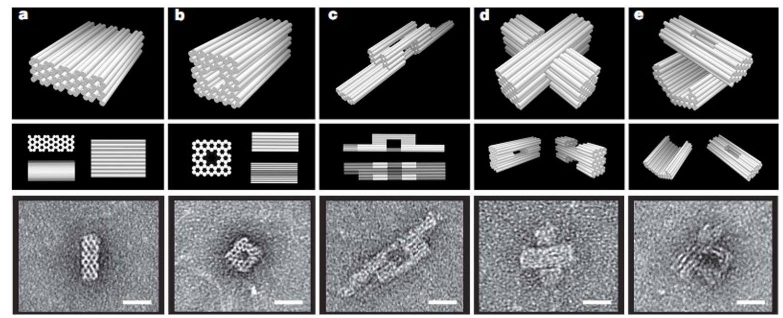
2006



Folding DNA To Create Nanoscale Shapes And Patterns: Rothemund

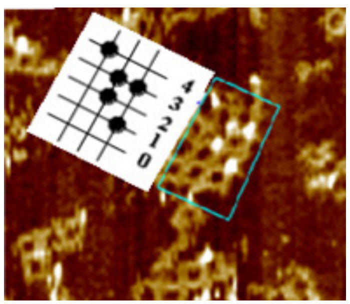
2009

Harvard



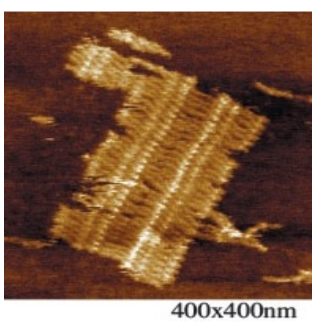
Self-assembly Of DNA Into Nanoscale Three-dimensional Shapes: Douglas, Dietz, Liedl, Hogberg, Graf, Shih

Duke



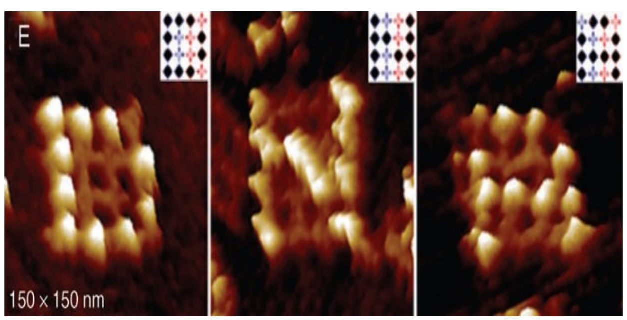
Unpublished Data: Majumder, Reif

2003



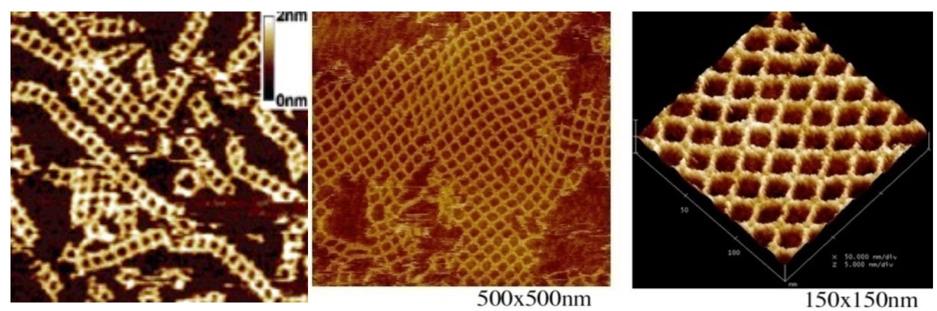
Directed Nucleation Assembly Of DNA Tile Complexes For Barcode-patterned Lattices: Yan, Labean, Feng, Reif

2006



Finite-size, Fully-addressable DNA Tile Lattices Formed By Hierarchical Assembly Procedures : Park, Pistol, Ahn, Reif, Lebeck, Dwyer, Labean

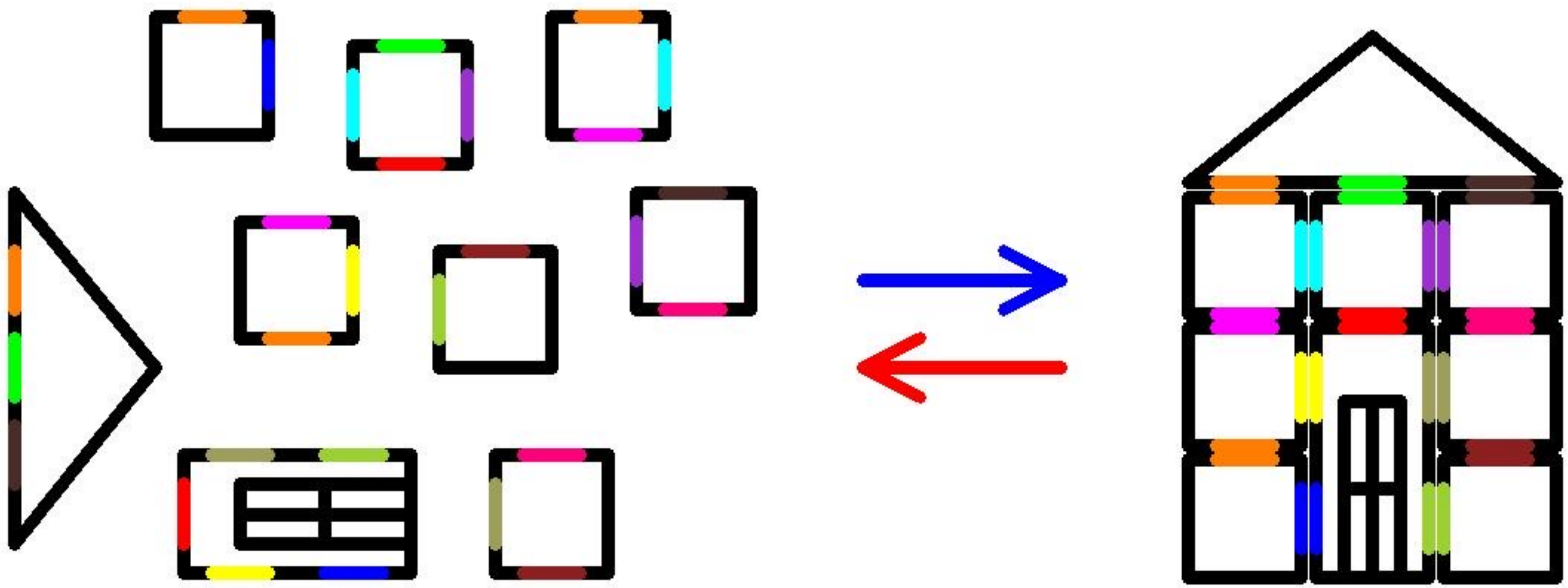
2003



4x4 DNA Tile And Lattices: Characterization, Self-assembly And Metallization Of A Novel DNA Nanostructure Motif : Yan, Park, Finkelstein, Reif And Labean

Introduction to Tile Self-Assembly

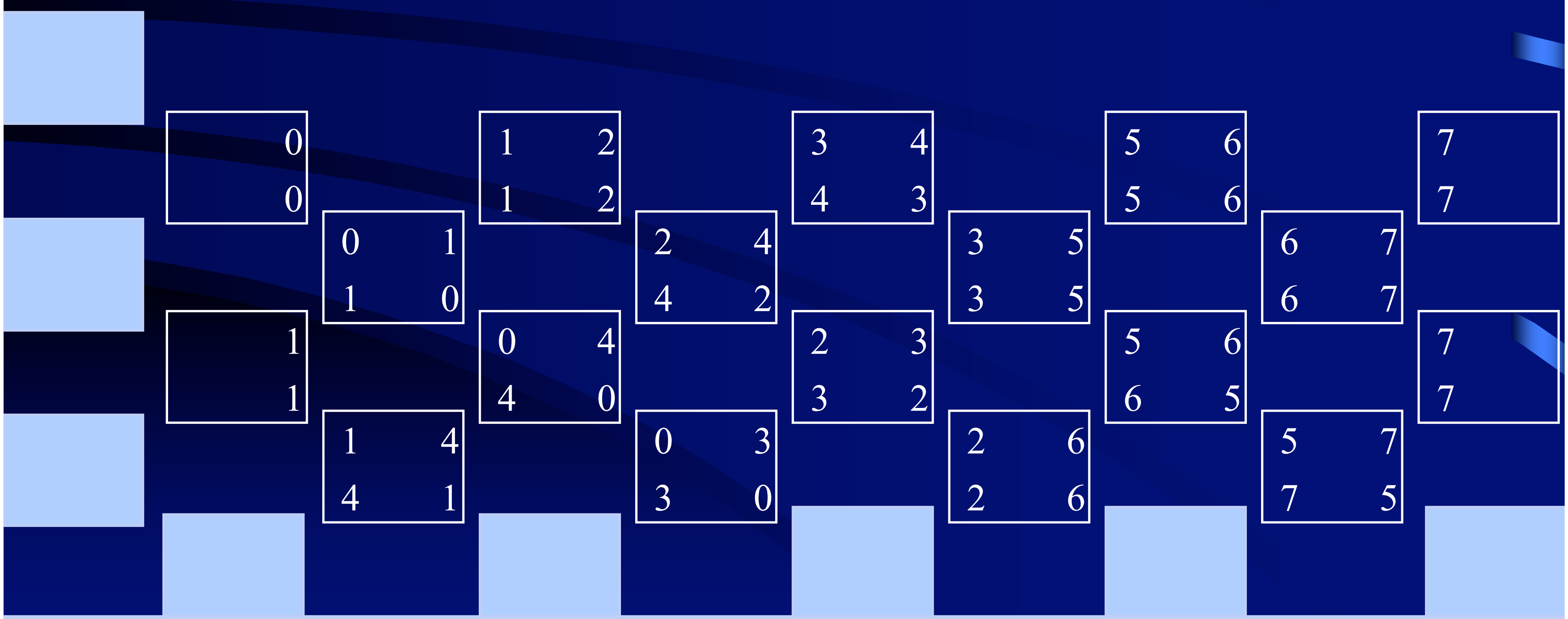
Construction with "*Smart*" Building Blocks



A tiling assembly using `Smart Bricks' with affinity between colored pads.

Computation with "Smart Bricks"

Sorting



A tiling assembly using `Smart Bricks' to Sort 8 Keys.

Scales of Tiling Assemblies:

- **Meso-Scale Tiling Assemblies:**
  - have tiles of size a few millimeters up to a few centimeters.
- **Molecular-Scale Tiling Assemblies:**
  - have tiles of size up to a few hundred Angstroms.

Tile Pad Binding Mechanisms

Used for the preferential matching of tile sides

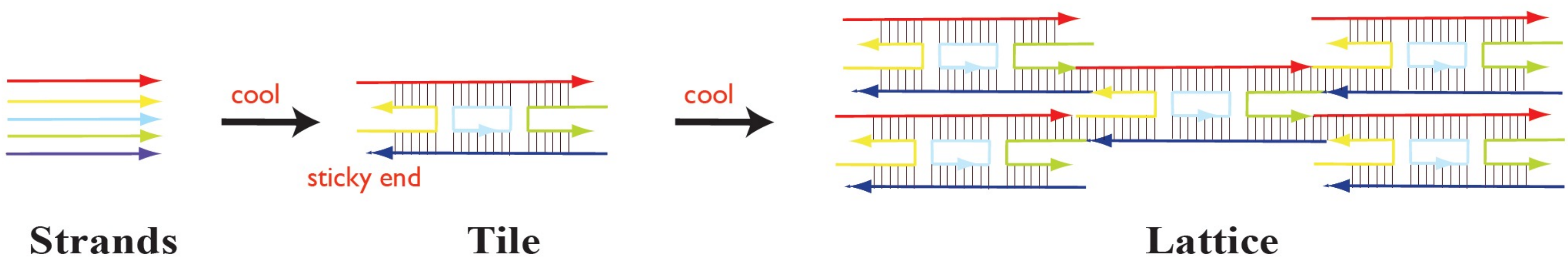
- Molecular Affinity (Seeman, NYU): **Molecular-Scale**
  - **hydrogen bonding of complementary DNA or RNA bases**
- Magnetic Attraction (Univ Wisconsin): **Meso-Scale**
  - **pads with magnetic orientations constructed by curing polymer/ferrite composites in the presence of strong magnet fields, or**
- **pads with patterned strips of magnetic orientations [Reif].**
- Shape Complementarity: [Whitesides, Harvard U]: **Meso-Scale**
  - **using the conformational shape affinity of the tile sides to hold them together.**
- Capillary Force [Whitesides, Harvard U], [Rothmemund, 1999]: **Meso-Scale**
  - **using hydrophobic/hydrophilic (capillary) effects at surface boundaries that generate lateral forces.**

Design & Experimental Demonstration of DNA Tiles and Lattices

Self-assembly of DNA lattices

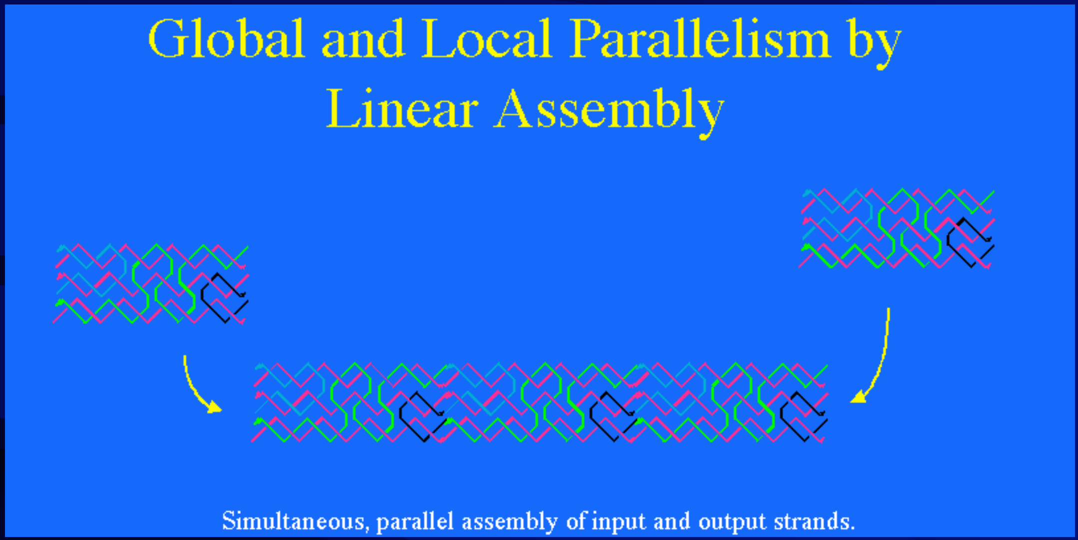
- Driven by Watson-Crick base pairing : A ↔ T & C ↔ G
- Leads to energy minimization of the final structure
  - Base pairing and base stacking
- Programmability:
  - AGTGC sticks to GCACT (reverse complement)

Self-Assembly from DNA strands, to Tiles, to Lattices:



Programming Self-assembly of DNA Tilings = Design of Pads of DNA Tiles.

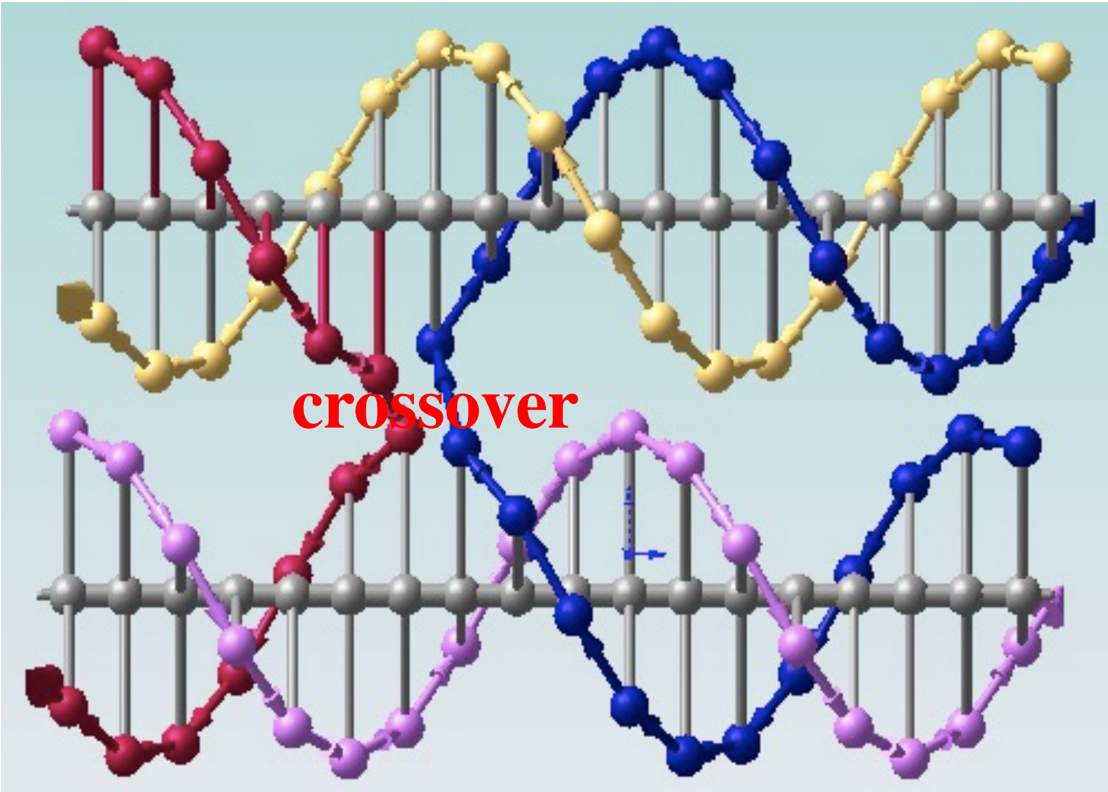
- Pads: complementary base sequences determining neighbor relations of tiles in final assembly
- Large-Scale Computational Tilings formed during assembly:
  - encode valid mappings of input to output.
  - local tile association rules insure only valid computational lattices form regardless of temporal ordering of binding events.



- Key Advantageof DNA Self-Assembly for DNA Computing:
  - Use a sequence of only 4 laboratory procedures:
    - mixing the input oligonucleotides to form the DNA tiles,
    - allowing the tiles to self-assemble into superstructures,
    - ligating strands that have been co-localized, and
    - performing a single separation to identify the correct output.

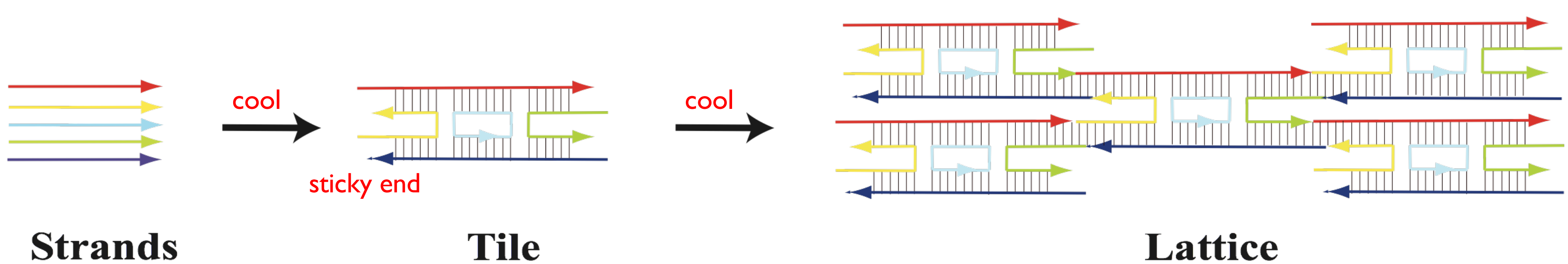
DNA tiles

DNA molecules self-assembled from artificially synthesized single stranded DNA.



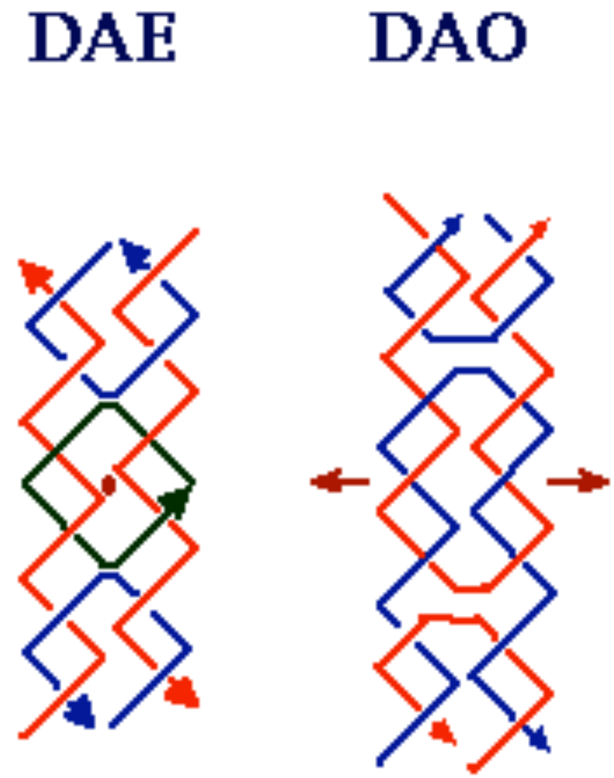
- **Anti-parallel crossovers:**
  - **cause a reversal in direction of strand propagation through the tile following exchange of strand to a new helix.**
- **Pads:**
  - **Tiles have sticky ends that preferentially match the sticky ends of certain other DNA tiles.**
  - **The sticky ends facilitate the further assembly into tiling lattices.**

Self-Assembly from DNA strands, to Tiles, to Lattices:



DNA Tiles:

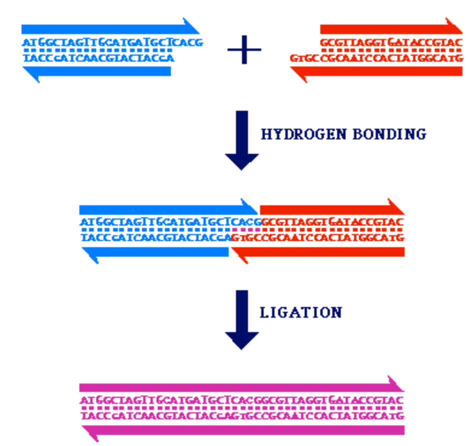
Are DNA crossover molecules self-assembled from artificially synthesized single stranded DNA.



Double-crossover (DX) Tiles [Winfree, Seeman]:

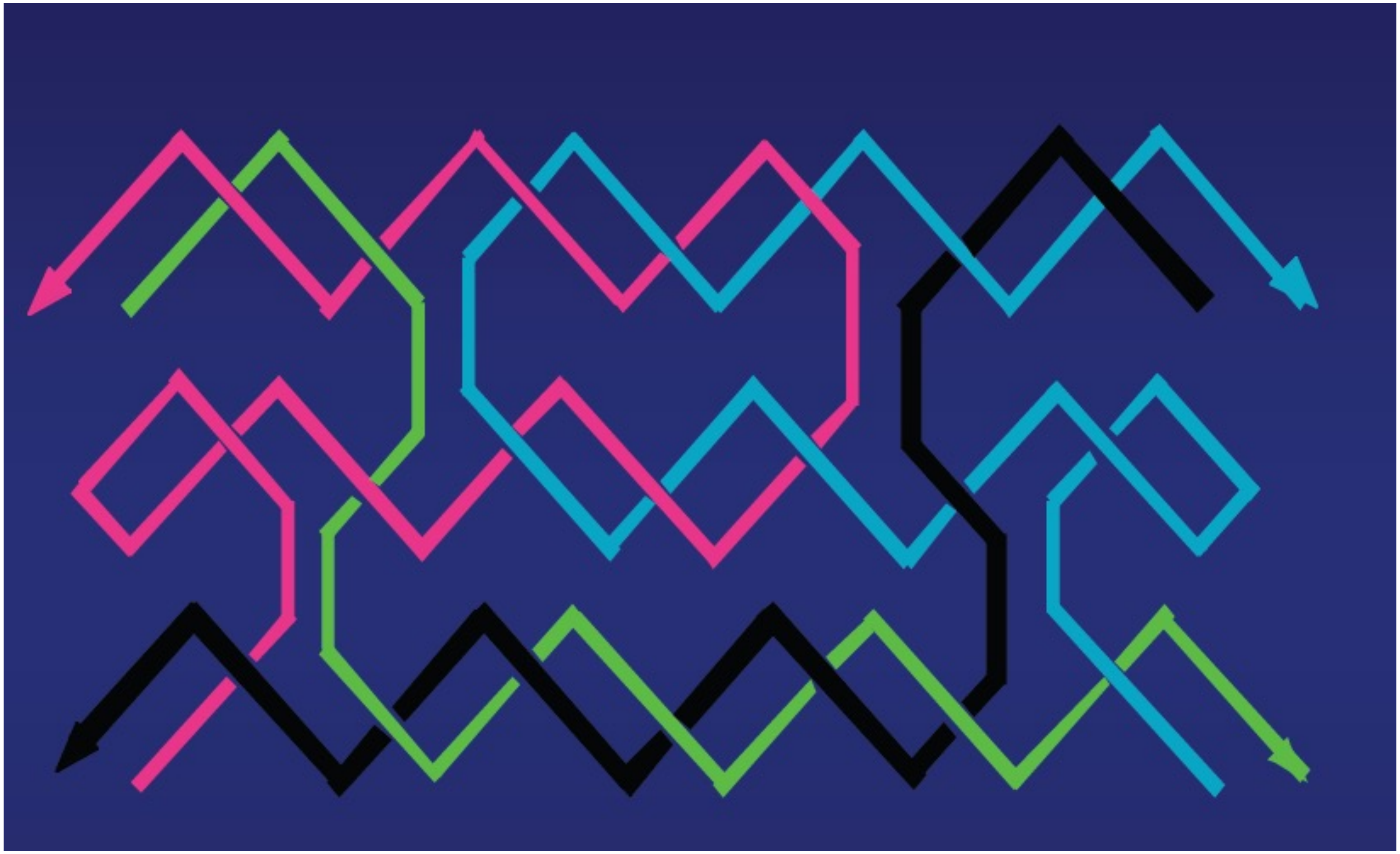
- **consist of two double-helices fused by crossover**
- **DAE contains an Even number of helical half-turns between crossover points.**
- **DAO contains an Odd number.**

- **Anti-parallel crossovers:**
  - **cause a reversal in direction of strand propagation through the tile following exchange of strand to a new helix.**
  - **DAO and DAE are double-crossover DX tiles with two anti-parallel crossovers.**
- **Pads:**
  - **Tiles have sticky ends that preferentially match the sticky ends of certain other DNA tiles.**
  - **The sticky ends facilitate the further assembly into tiling lattices.**
  - **Total of 4 Pads of single stranded DNA at ends.**

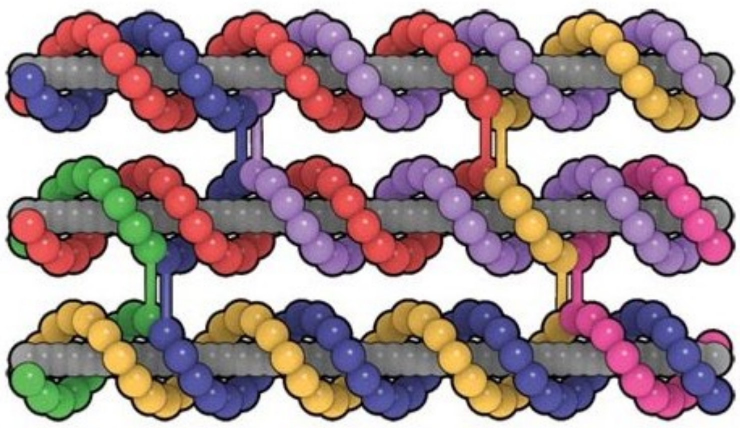


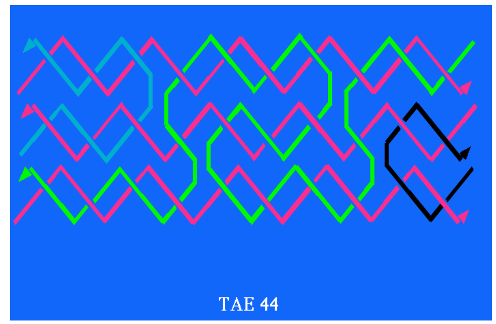
Triple Crossover (TX) Tiles

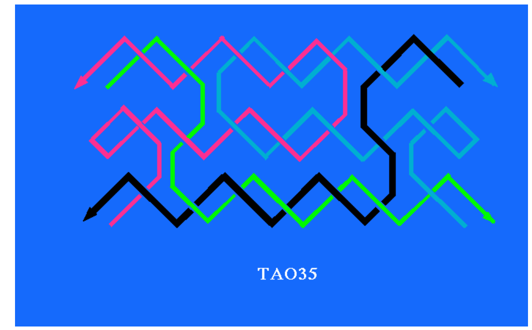
- **Is extension of the DX tile**
- **TX has 3 DNA helices made of 4 strands**

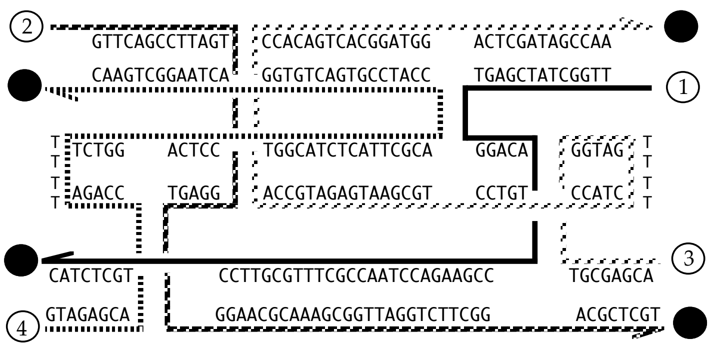


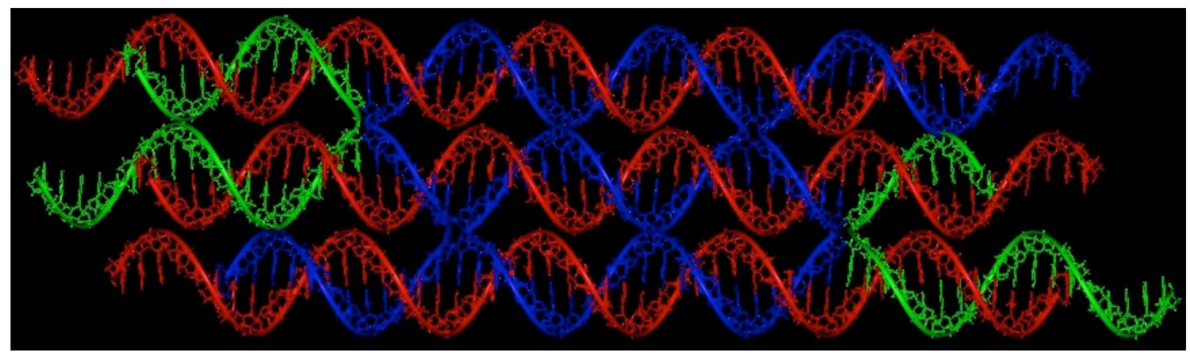
TX Tiles







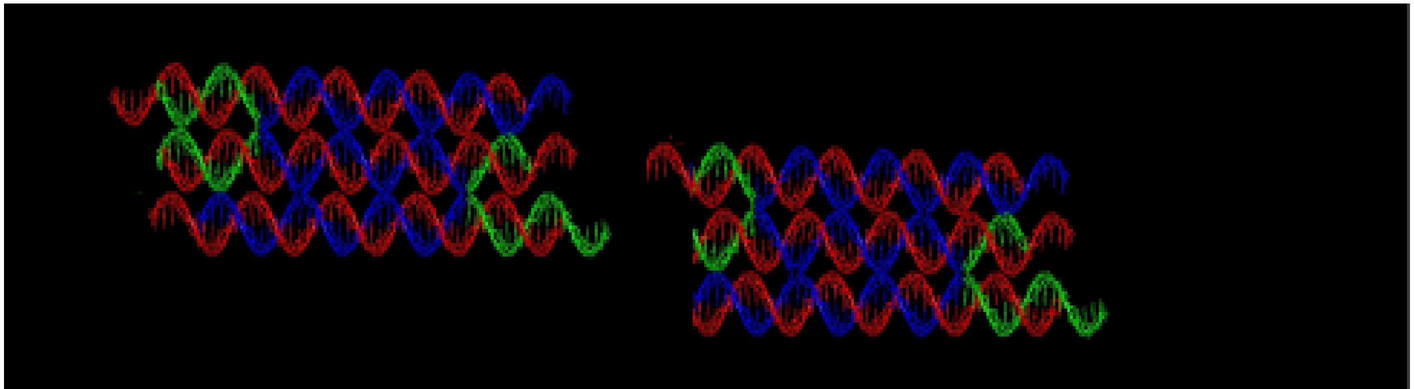




Triple-crossover (TX) Tiles [LaBean, Reif et al, J. Am. Chem. Soc., 2000]:

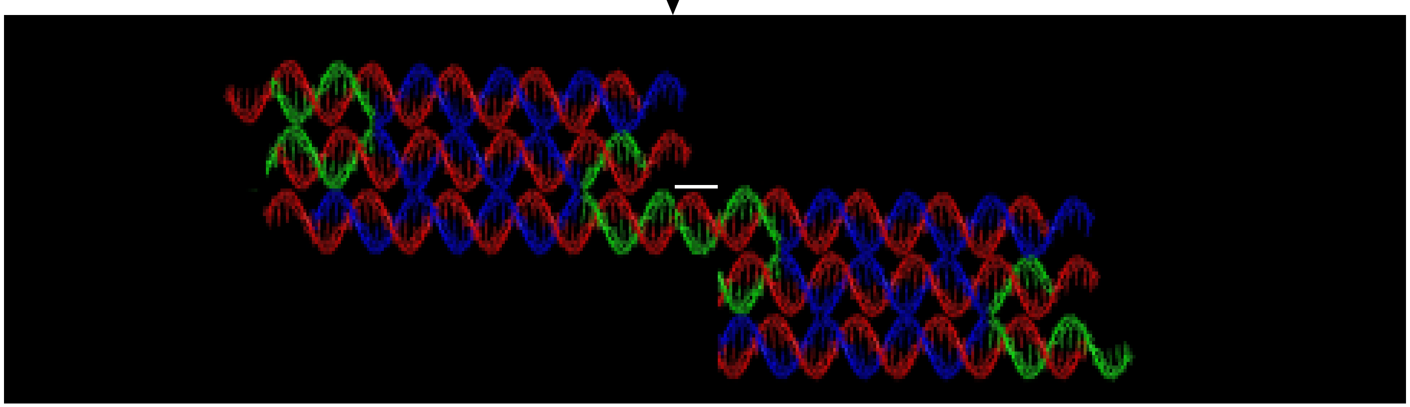
- consist of three double-helices fused by crossover strands.
- TAE contains an Even number of helical half-turns between crossover points.
- TAO contains an Odd number.
- Total of 6 Pads of single stranded DNA at ends.

Unique Sticky Ends on DNA tiles. Input layers can be assembled via unique sticky-ends at each tile joint thereby requiring one tile type for each position in the input layer.



Tiling self-assembly:

proceeds by the selective annealing of the pads of distinct tiles, which allows tiles to compose together to form a controlled tiling lattice.



DNA Tile Design Software

DNA Tile Design Software

- **Why do we need DNA sequence optimization?**

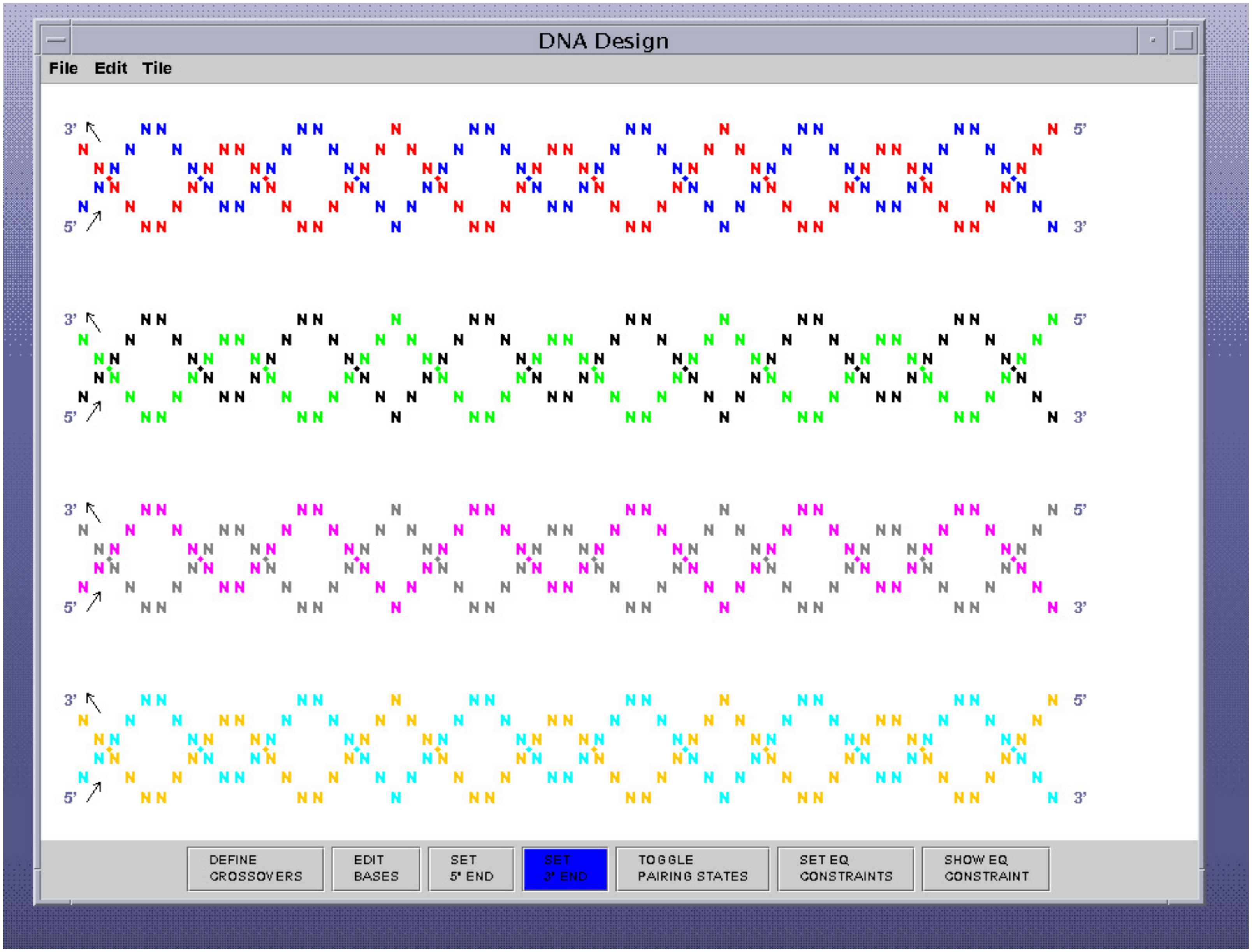
- ***DNA-Design* Software by Winfree (Random Search Algorithm)**

- **Improved with Evolutionary algorithm**

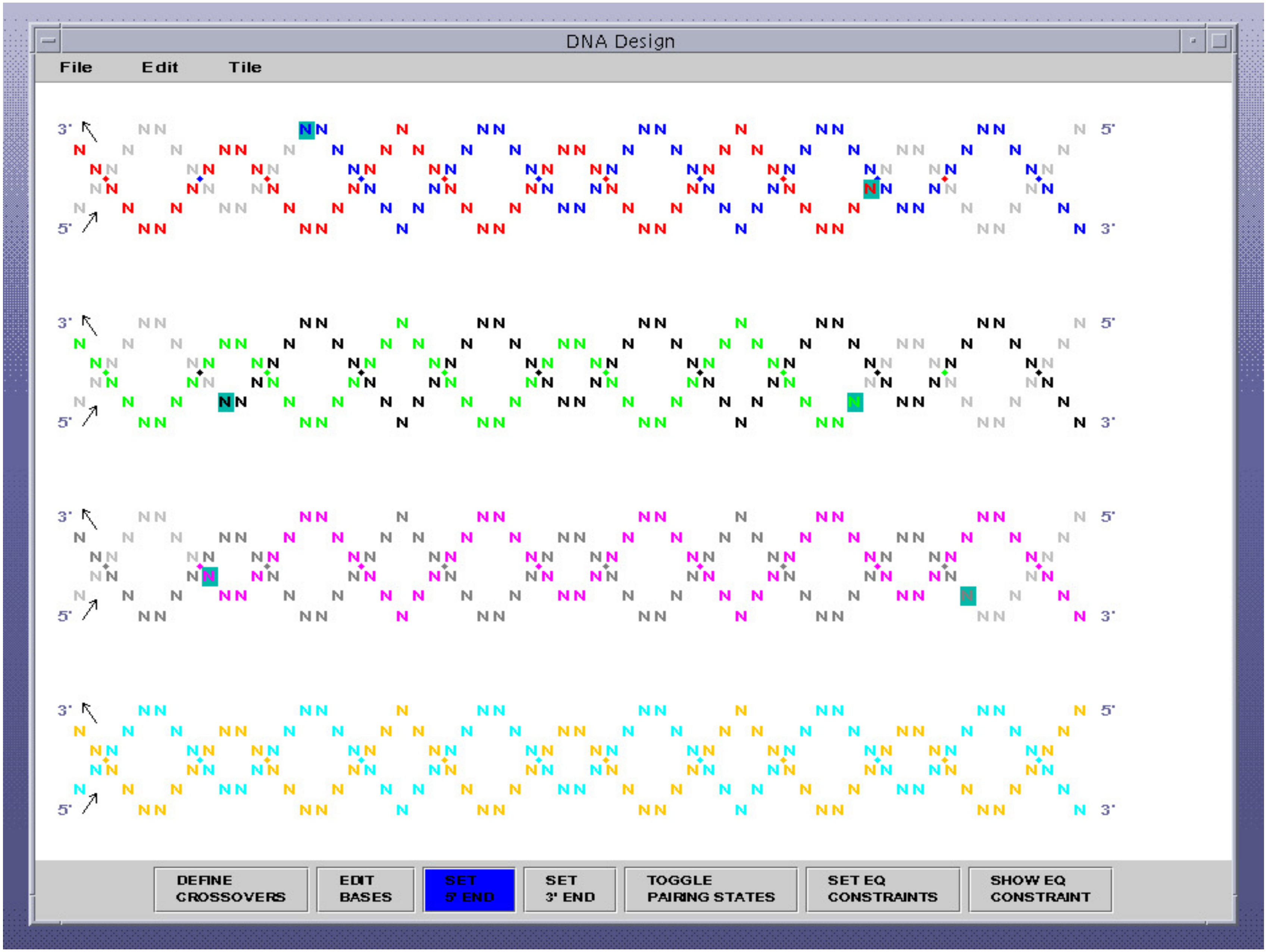
=

- **Graphical User Interface**

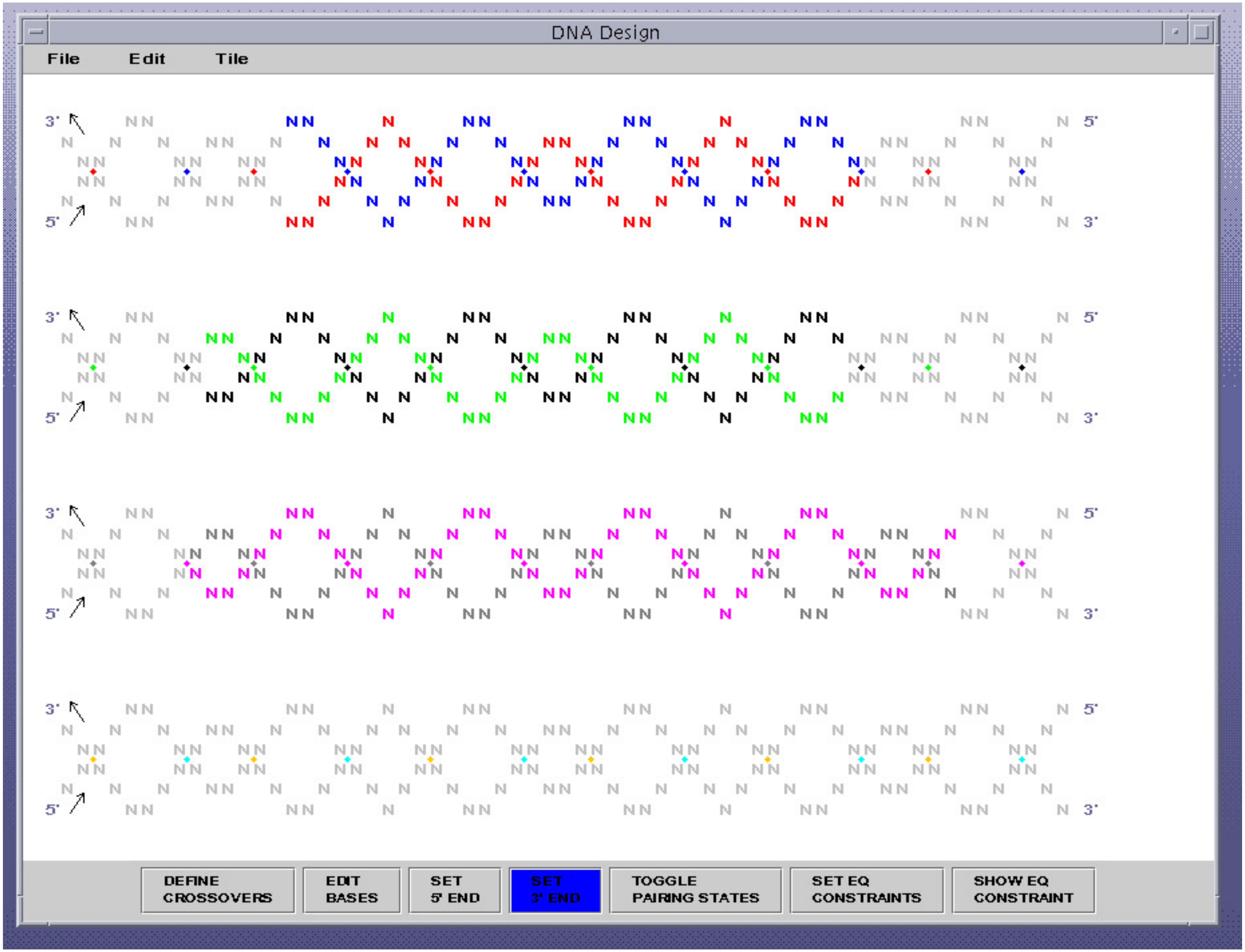
Software Interface



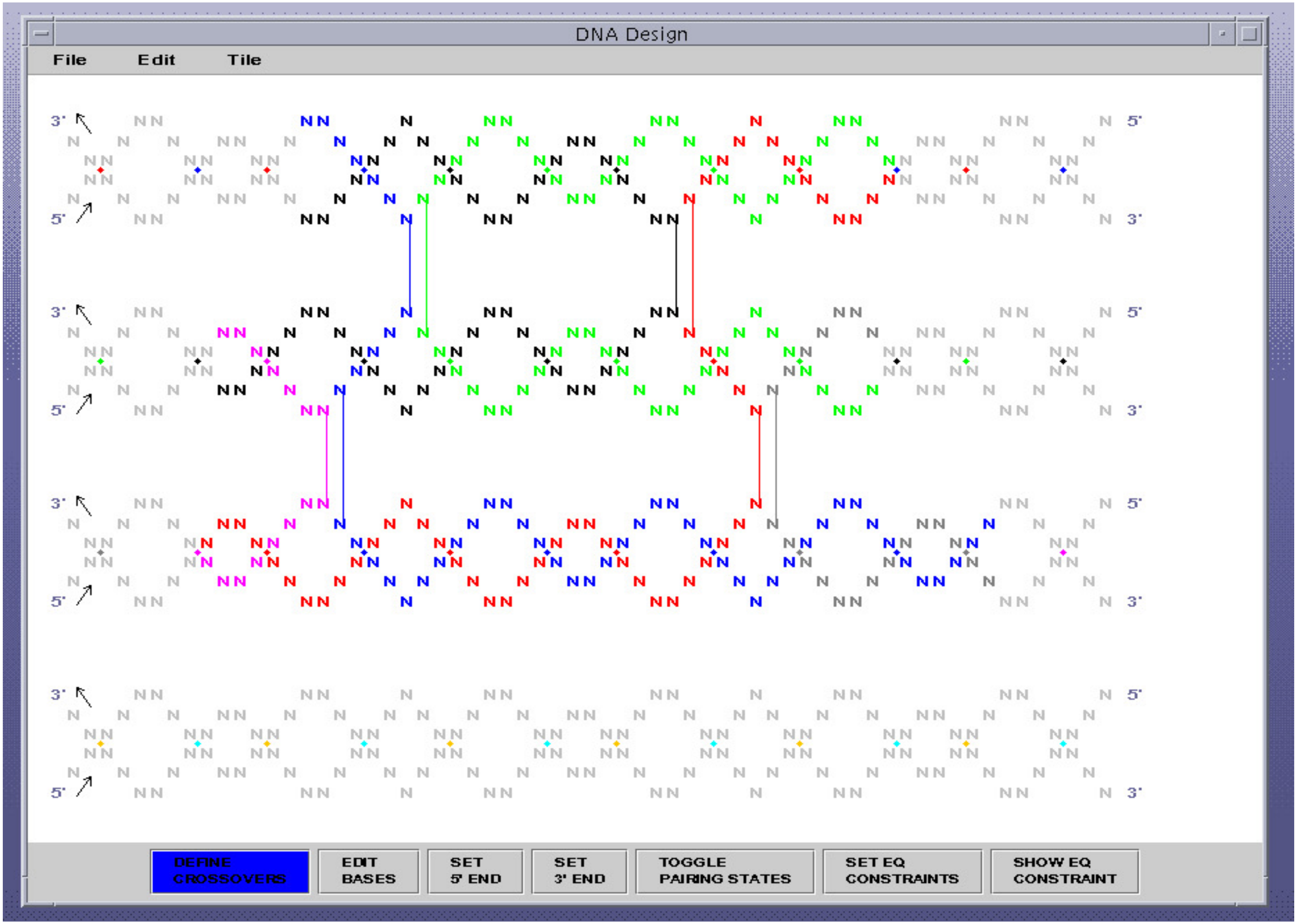
Setting 5' end



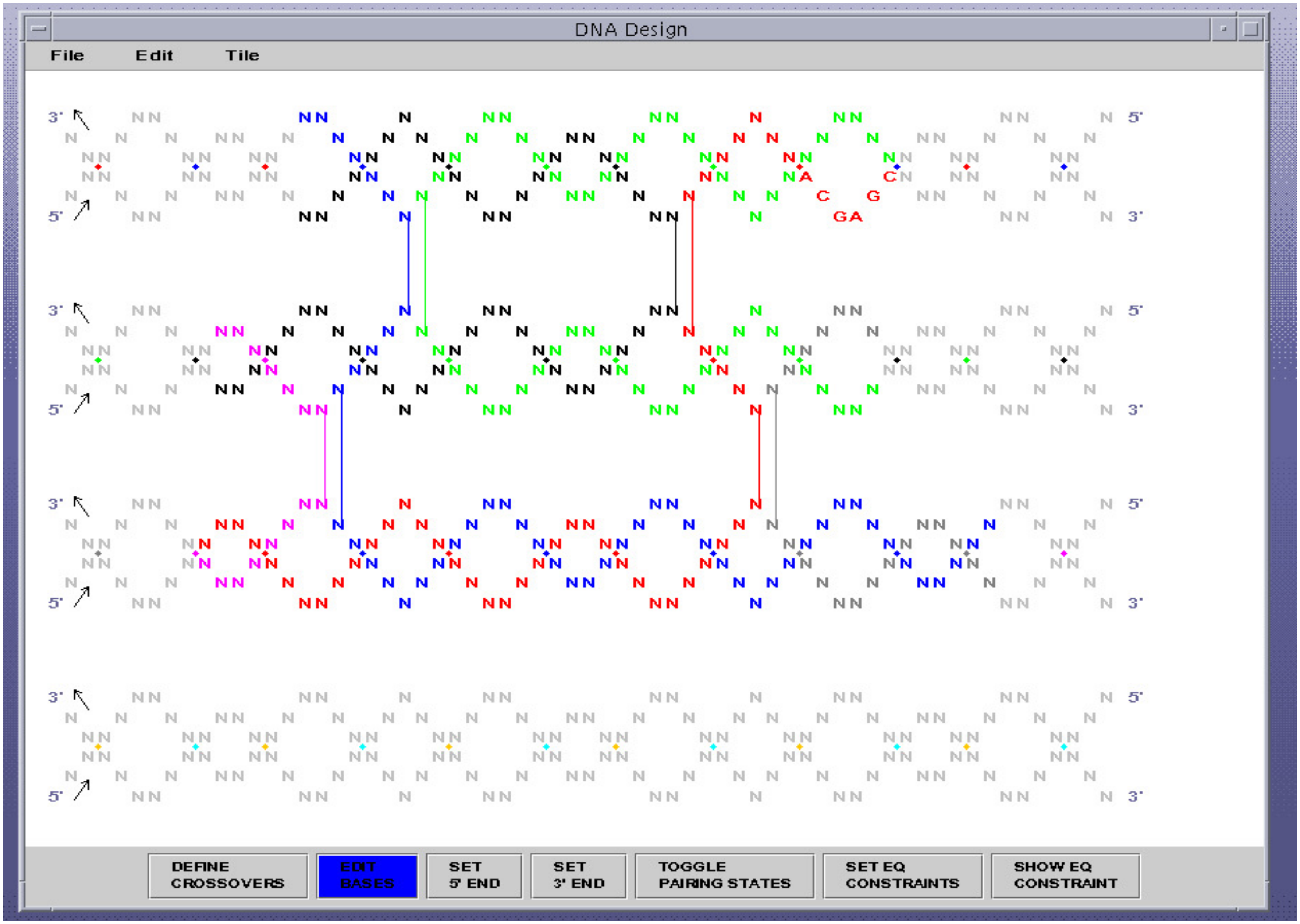
Setting 3’ end



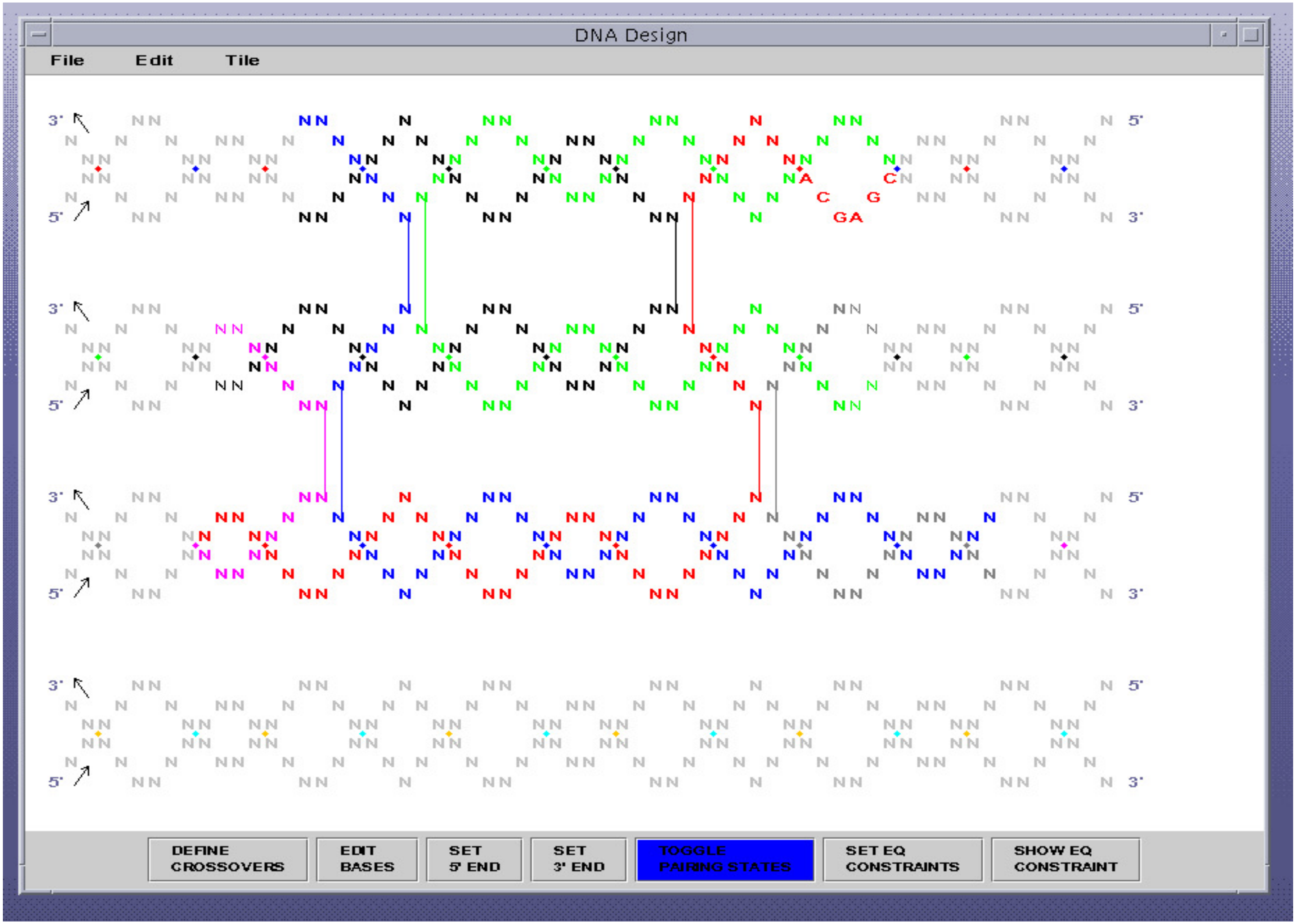
Defining Junctions



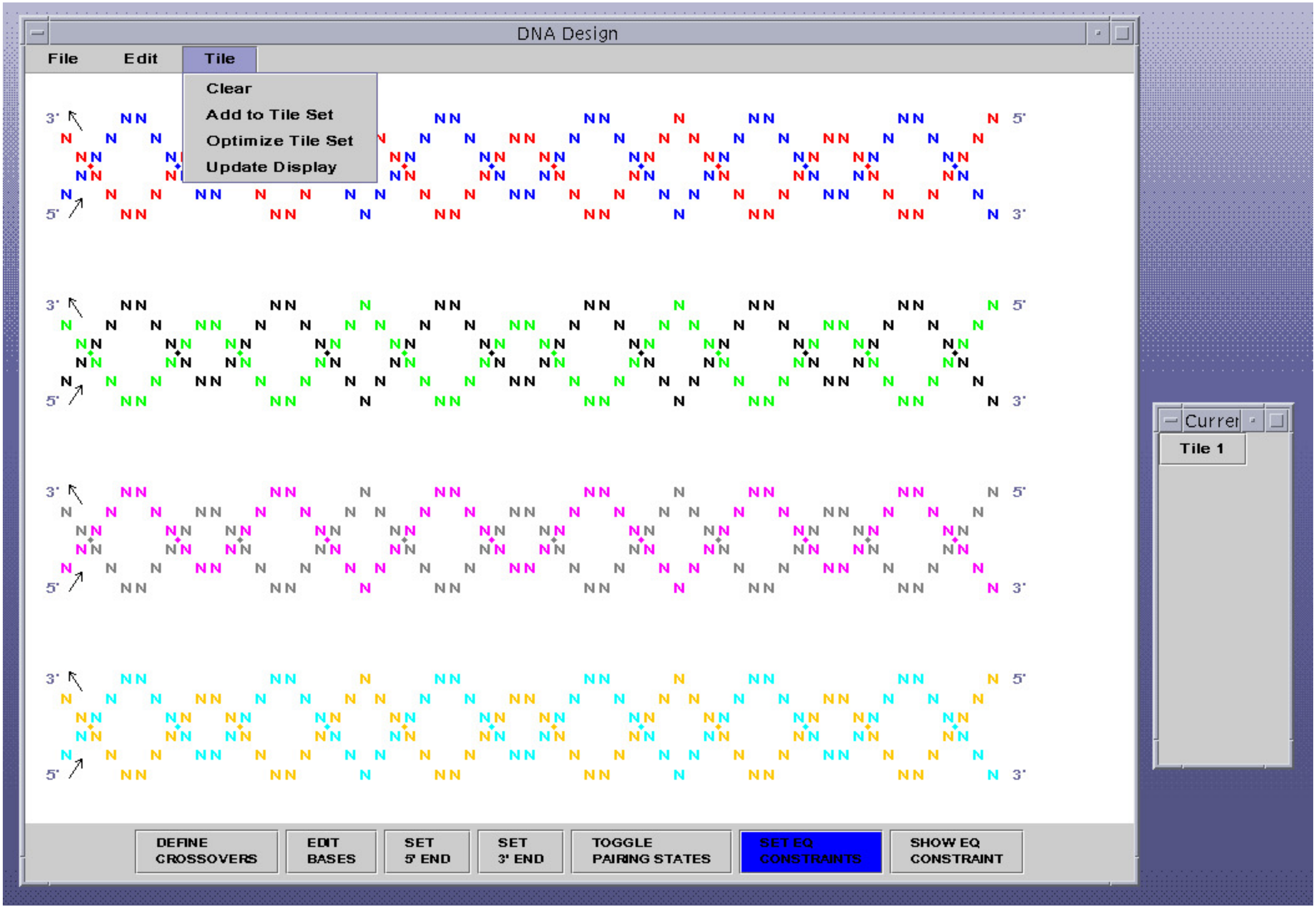
Editing Bases



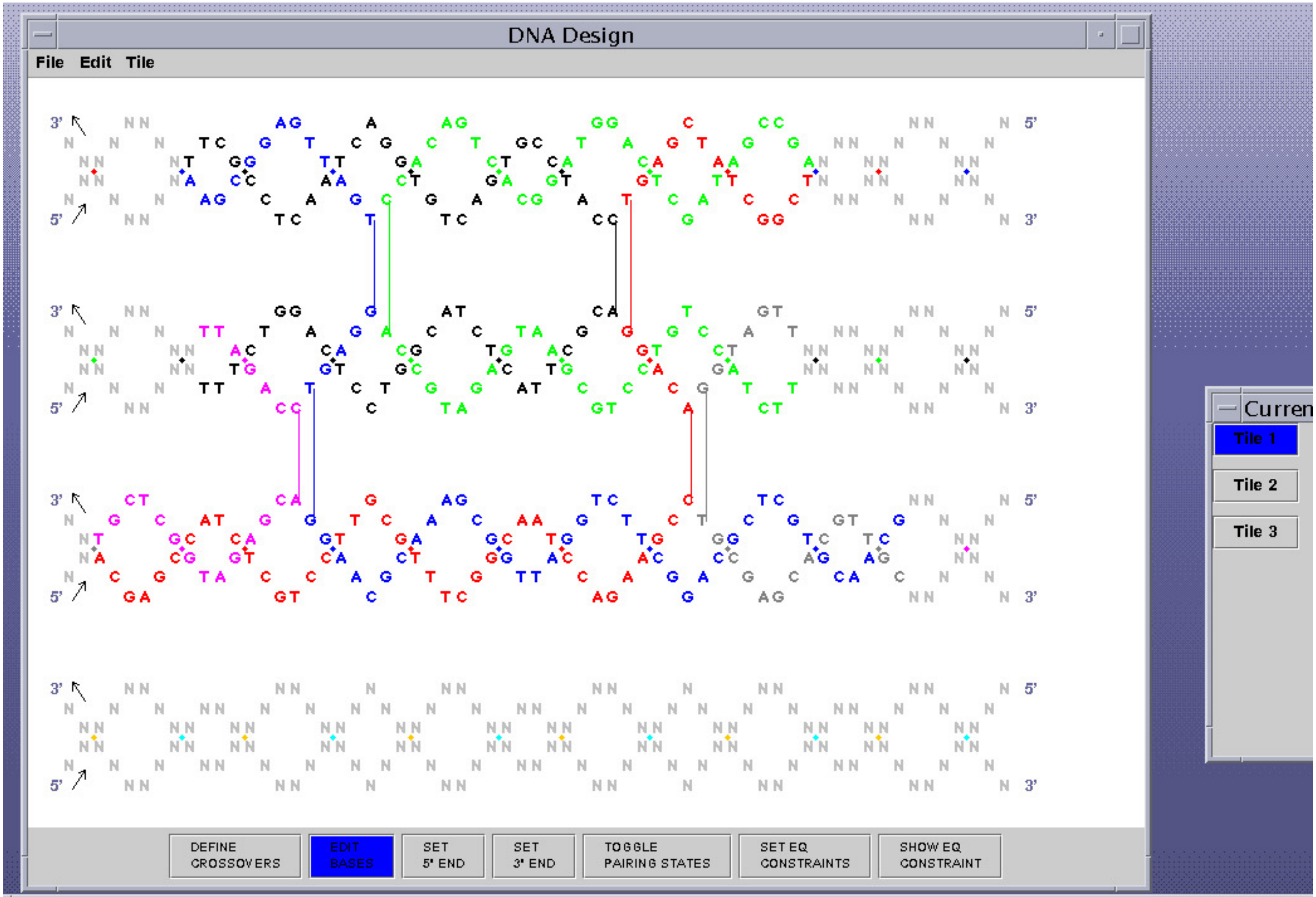
Setting WC constraints



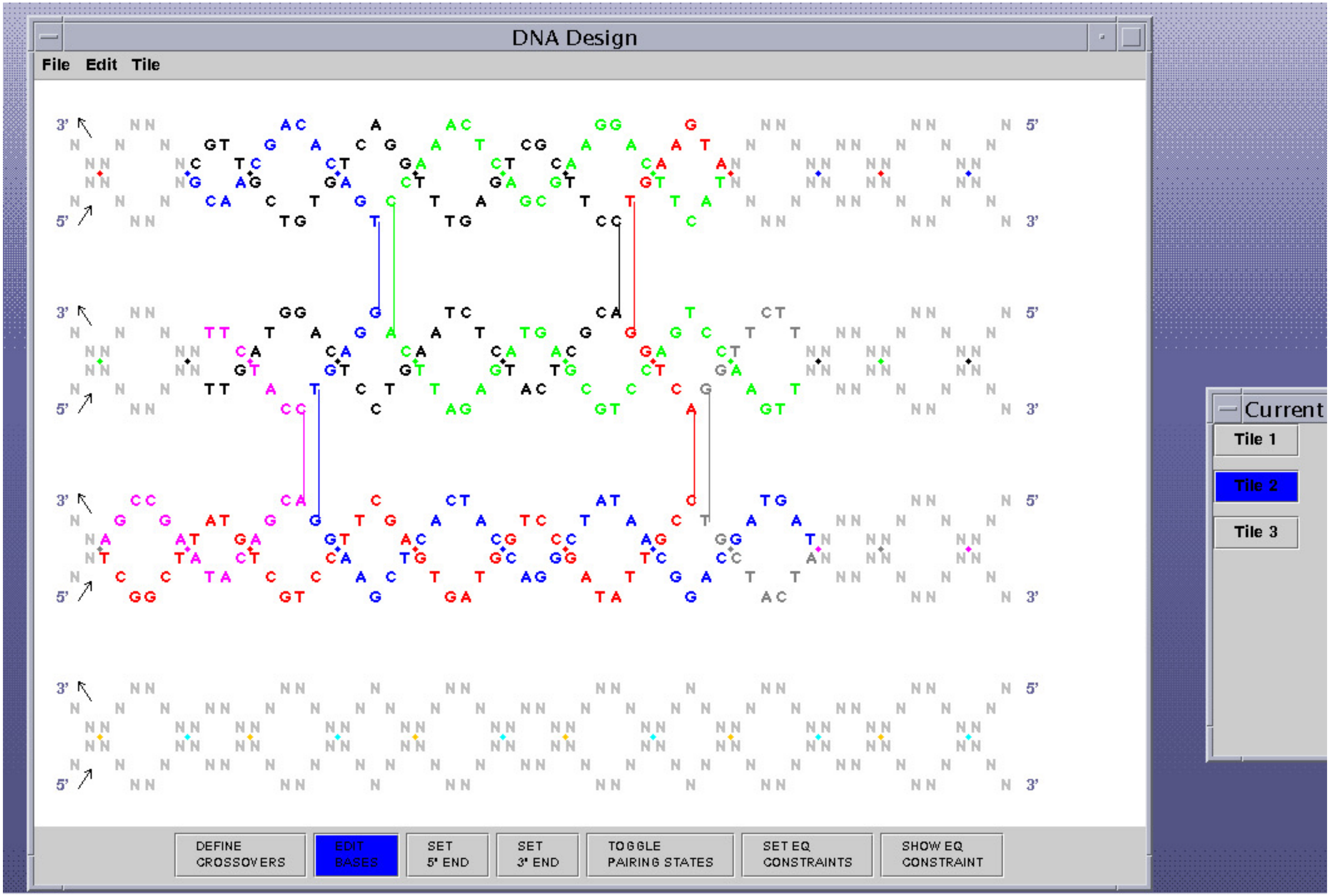
Adding the Tile to Tile Set



Tile A (Optimized)

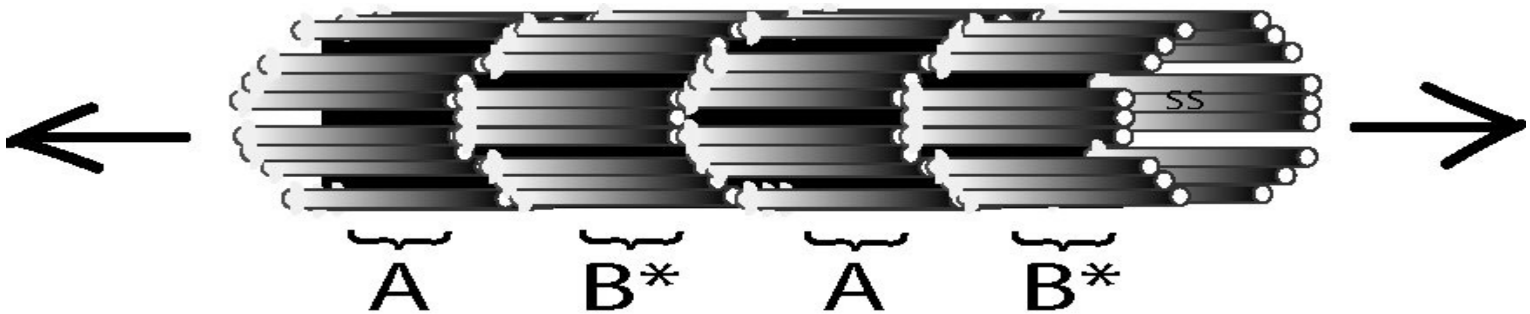


Tile B (Optimized)



Example: Designing C Tile for Nano-Barrel

[redacted]



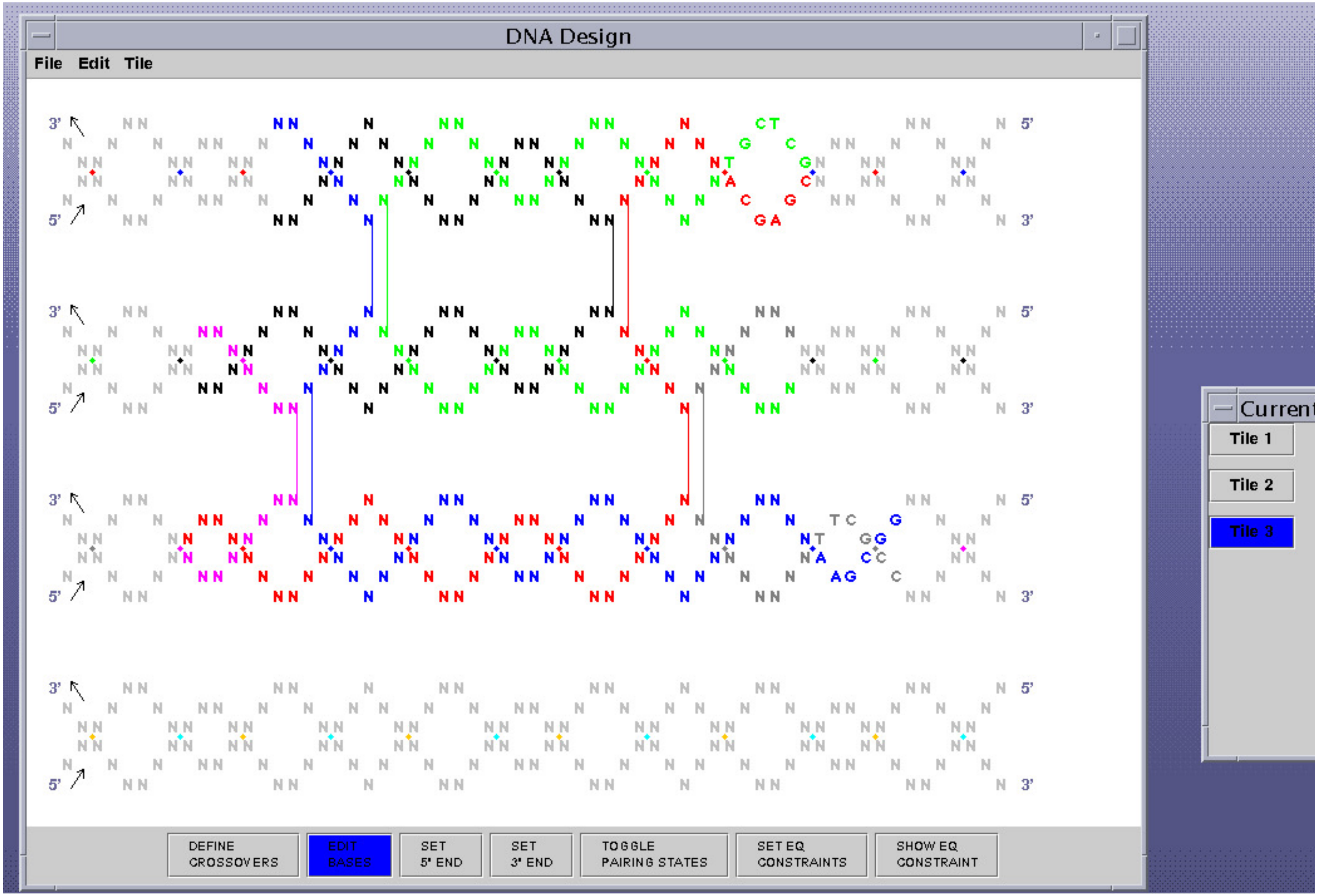
Task: Design C Tile

Task: Design C Tile

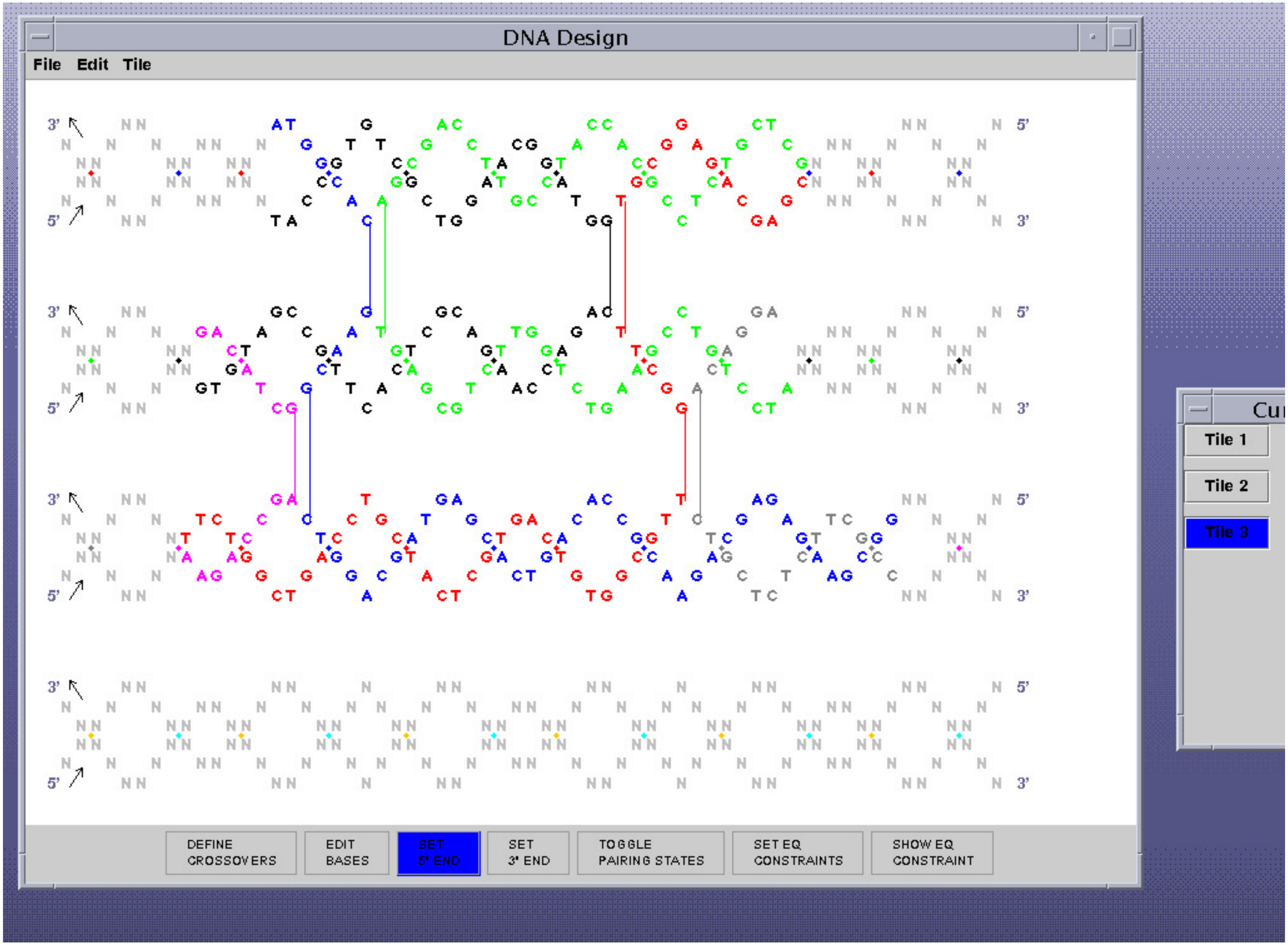
[redacted]

Figure Credit: Thomas. Labean

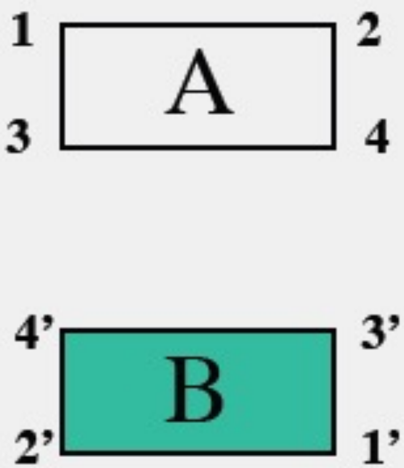
Tile C (To be optimized)

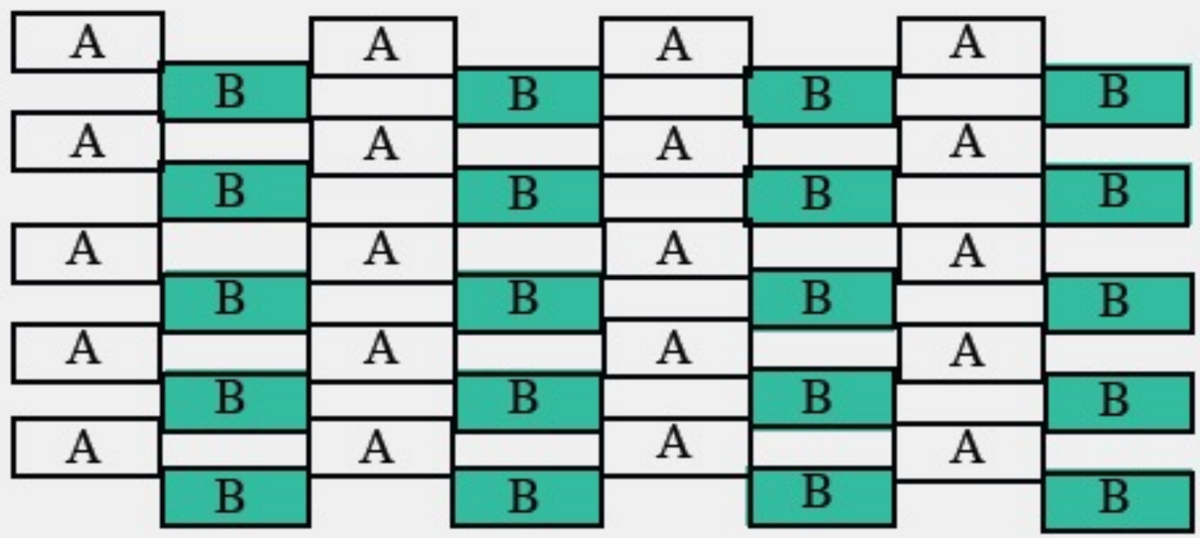


Tile C (Optimized)



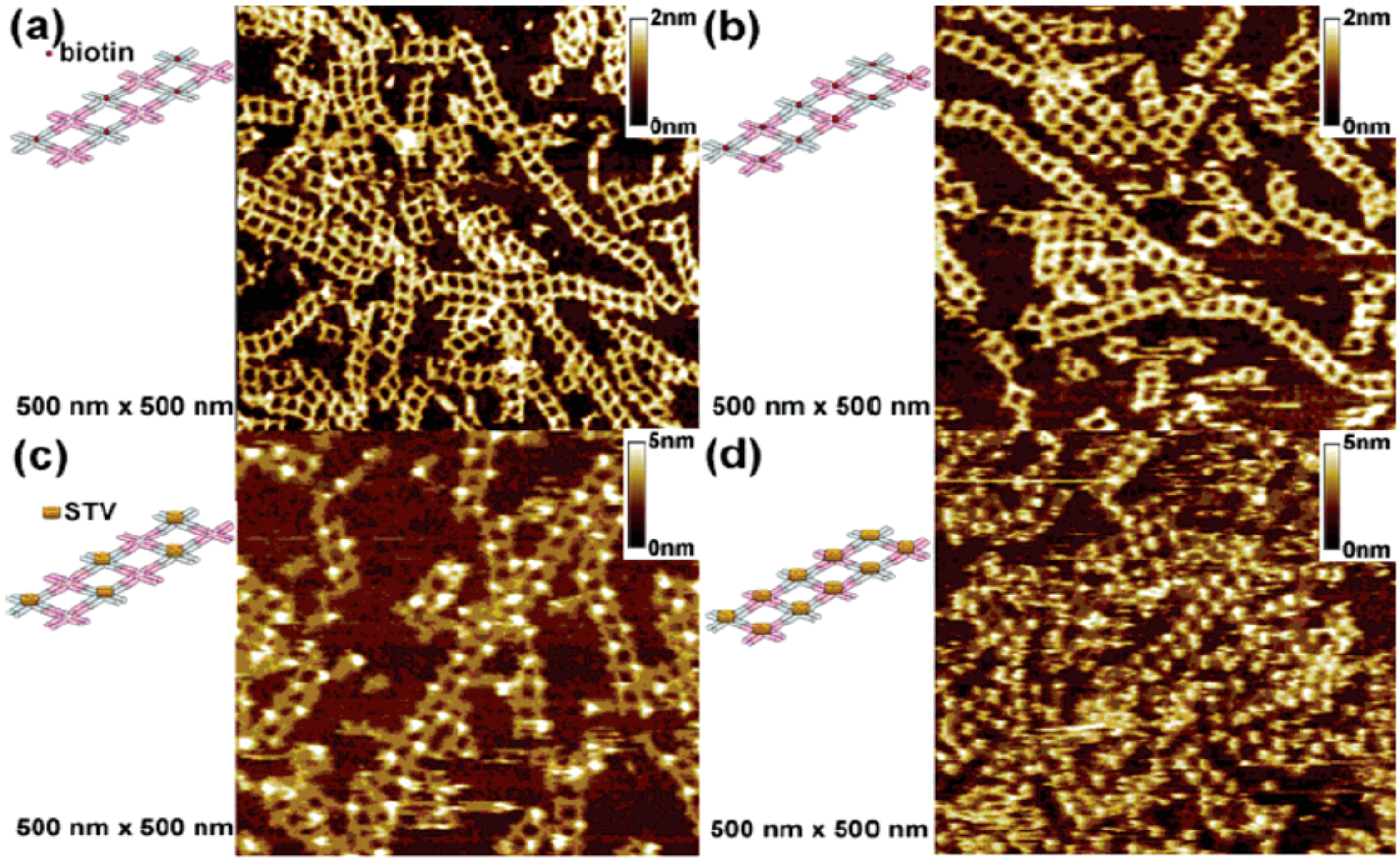
Lattices using TX Tiles





Linear DNA TX lattices with biotin covalently bound to DNA tiles

Can be used for patterning of heteromaterials using DNA-directed assembly.

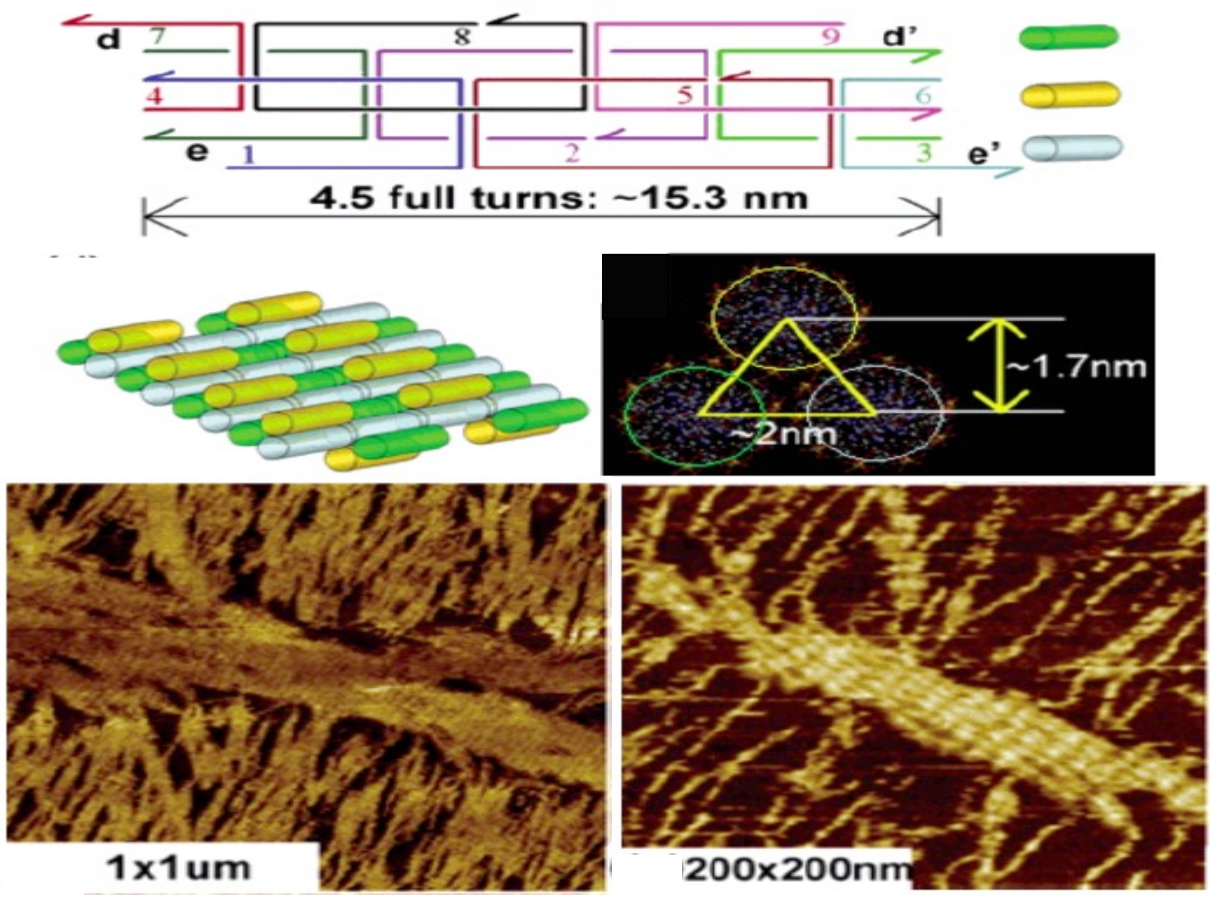


Sung Ha Park, Peng Yin, John Reif, Thomas LaBean, and Hao Yan, (2005) Programmable DNA Self-assemblies for Nanoscale Organization of Ligands and Proteins, *Nano Letters* 5(4) 729-733.

Three-helix bundle DNA tile Lattice

- Demonstrated for 1D and 2D self-assemblies
- Provides potential for tiling in the third dimension.
- The linear structures were used as templates for the electroless deposition of silver and formation of highly conductive silver nanowires with diameters of 20 – 30 nm.

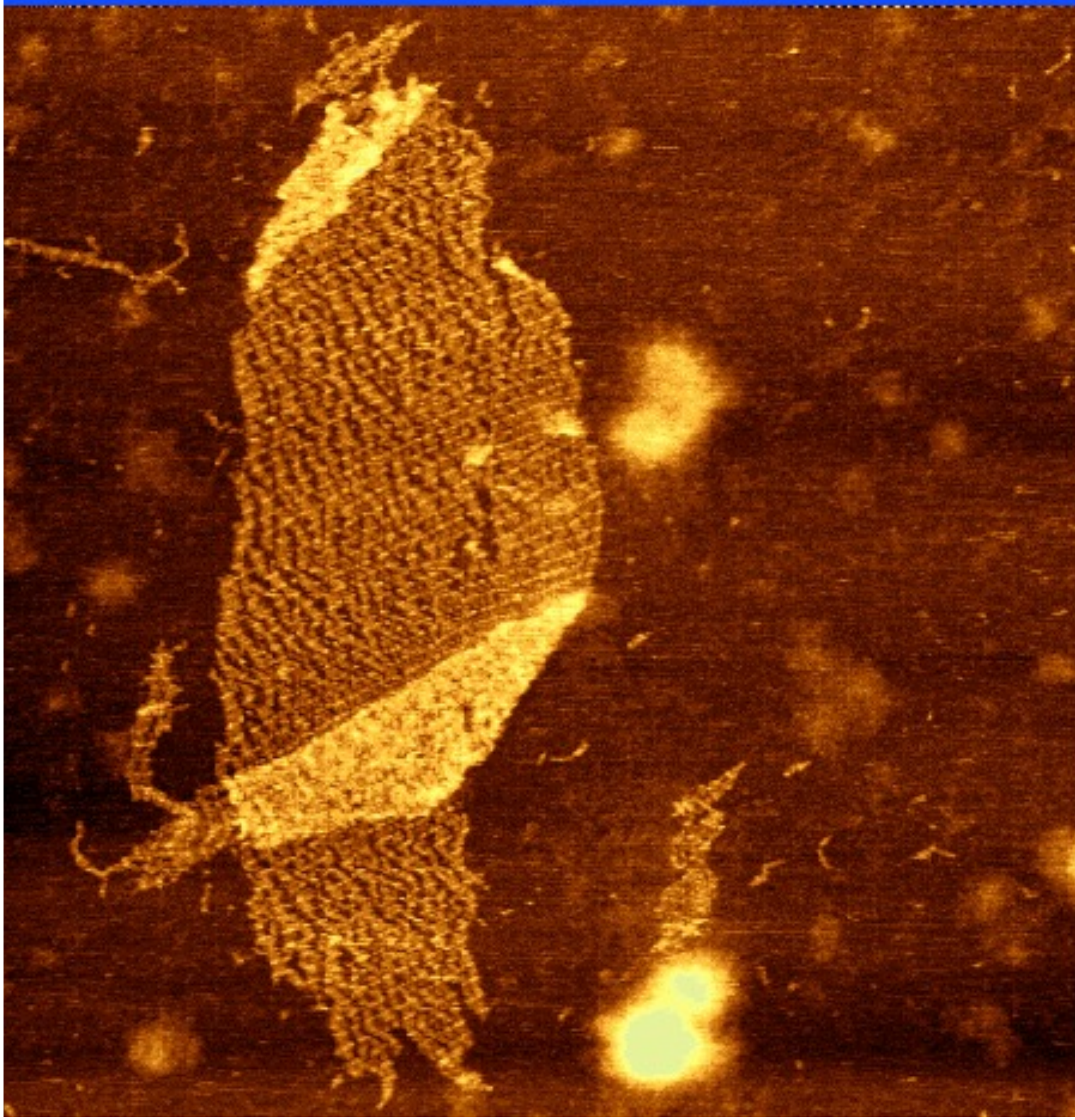
This tile type increases the toolbox of molecular building blocks with which to attack nano construction projects and patterning of heteromaterials using DNA-directed assembly.



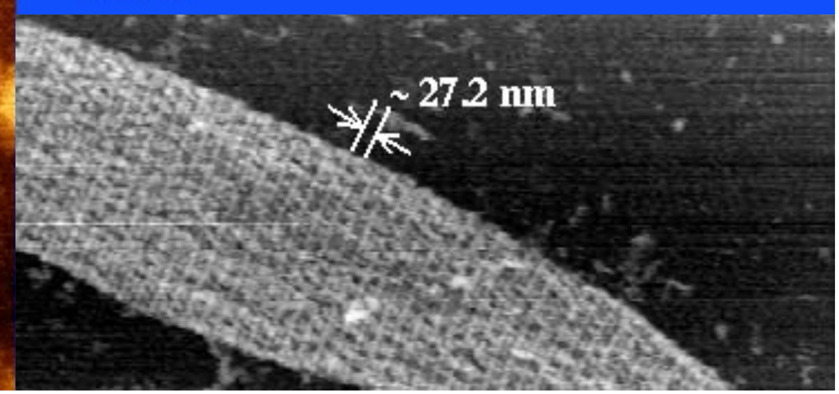
Sung Ha Park, Robert Barish, John Reif , Gleb Finkelstein, Hao Yan and Thomas LaBean, (2005) Three-Helix Bundle DNA Tiles Self-Assemble into 2D Lattice or 1D Templates for Silver Nanowires, *Nano Letters* 5(4) 693-696.

Large Scale DNA Self-Assembled Tilings

TX Lattice, with Visualization by Atomic Force Microscope.



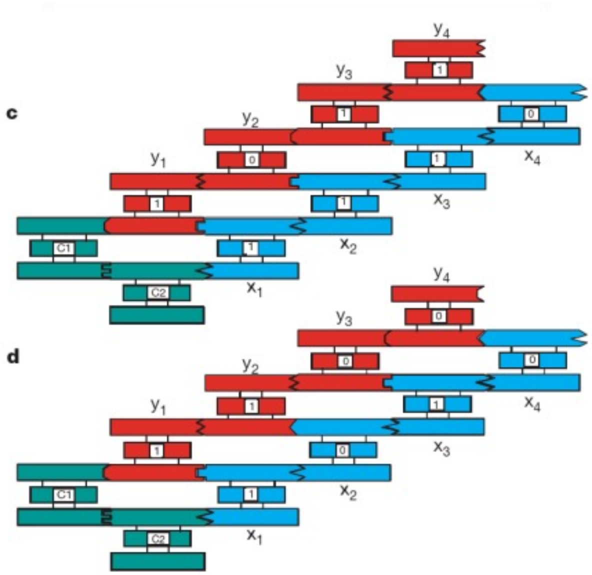
AB* Lattice. An atomic force microscope image of DNA lattice formed by two TAO tiles one of which contains an extra loop directed out of the plane. These loops form the visible stripe features with the expected spacing of ~28 nm.

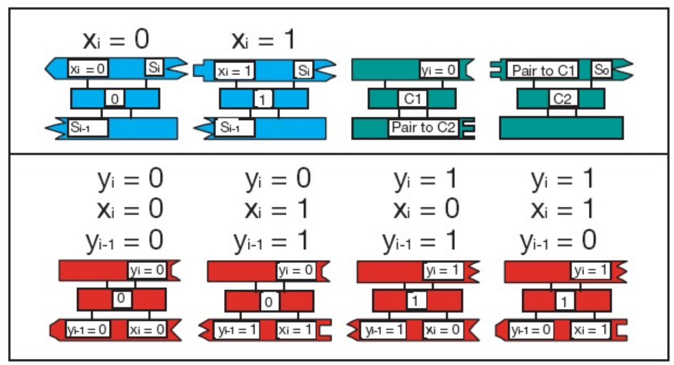


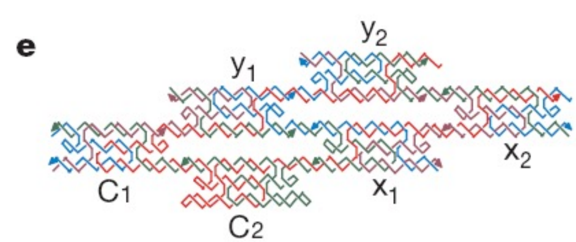
Computational DNA Lattices

Experimental Demonstrations of Molecular Computation via DNA Tiling

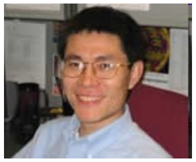
- First experimental demonstration of computation via molecular self-assembly: Computation of XOR using DNA triple-crossover molecules:
  - *Mao, LaBean, Reif, Seeman, Logical Computation Using Algorithmic Self-Assembly of DNA Triple-Crossover Molecules*







First Experimental Demonstration Computation via Tiling Assembly: 1D DNA Tiling Computation:

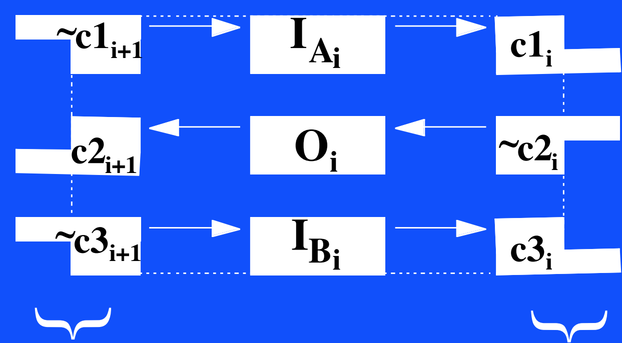


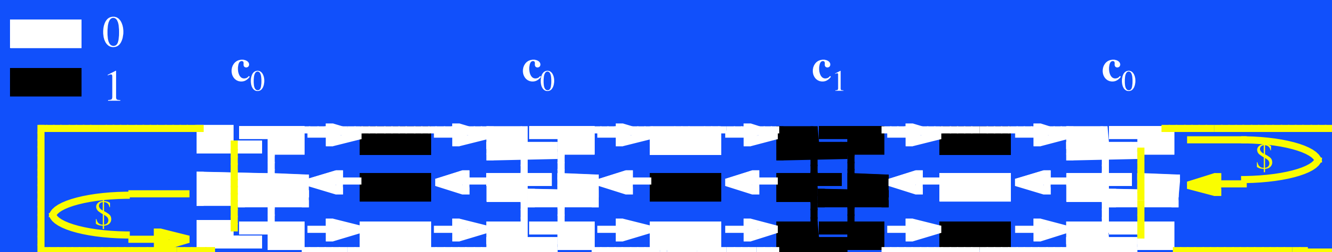
- C Mao, T H LaBean, J H Reif, N C Seeman, Logical Computation using Algorithmic Self-assembly of DNA Triple-crossover Molecules, *Nature* (2000)

- Hao Yan, Liping Feng, Thomas H. LaBean, and John Reif, Parallel Molecular Computations of Pairwise Exclusive-Or (XOR) Using DNA "String Tile" Self-Assembly, JACS (2003).

- **String Tile Addition Pads:**
  - The sticky end pads on right encode:
    - carry bits coming in and I_{Ai} and I_{Bi} encode the two input bits.
  - Left-hand pads pass new carry value on to next step
  - Reporter strands indicated by arrows; O_i encodes: output bit.

tile	c_i	I_{A_i}	I_{B_i}	O_i	c_{i+1}
1	0	0	0	0	0
2	0	0	1	1	0
3	0	1	0	1	0
4	0	1	1	0	1
5	1	0	0	1	0
6	1	0	1	0	1
7	1	1	0	0	1
8	1	1	1	1	1



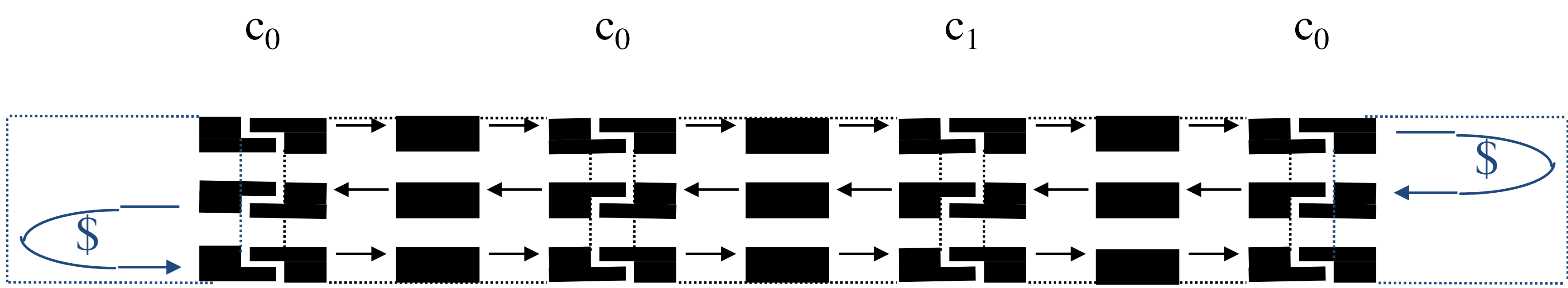


1 0 1 \$ 0 1 1 \$ 0 0 1 = I_A \$ O^R \$ I_B

$$\begin{array}{r} 101 \\ +\underline{001} \\ 110 \end{array}$$

- **Pad Programming via Truth Table:**
  - Column c_i gives values for the 3 right-hand pads ($c1_i$, $\sim c2_i$, $c3_i$)
  - Column c_{i+1} gives value for the 3 left-hand pads ($\sim c1_{i+1}$, $c2_{i+1}$, $\sim c3_{i+1}$).

“String Tile” Addition:



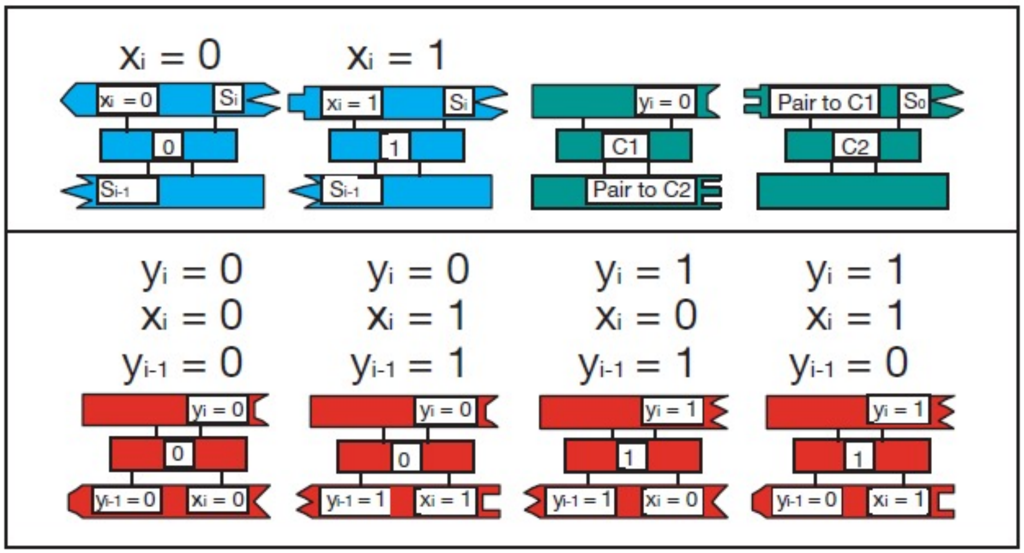
- Anneal strands to form assembly.
- Ligate reporter strand segments.
- Purify reporter strand and read values by PCR.

$$1\ 0\ 1\ \$\ 0\ 1\ 1\ \$\ 0\ 0\ 1 = I_A\ \$\ O^R\ \$\ I_B$$

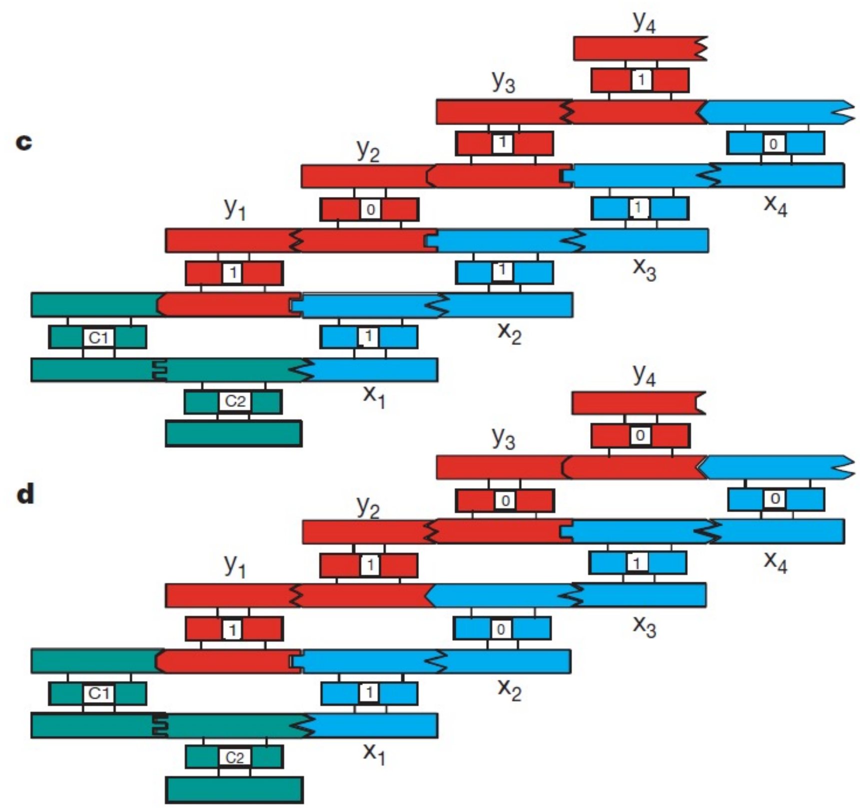
101
+001
110

Hao Yan, Liping Feng, Thomas H. LaBean, and John Reif, Parallel Molecular Computations of Pairwise Exclusive-Or (XOR) Using DNA "String Tile" Self-Assembly, JACS (2003).

The First Demonstration of Molecular Scale Computing using DNA Self-Assembly (TX tiles)



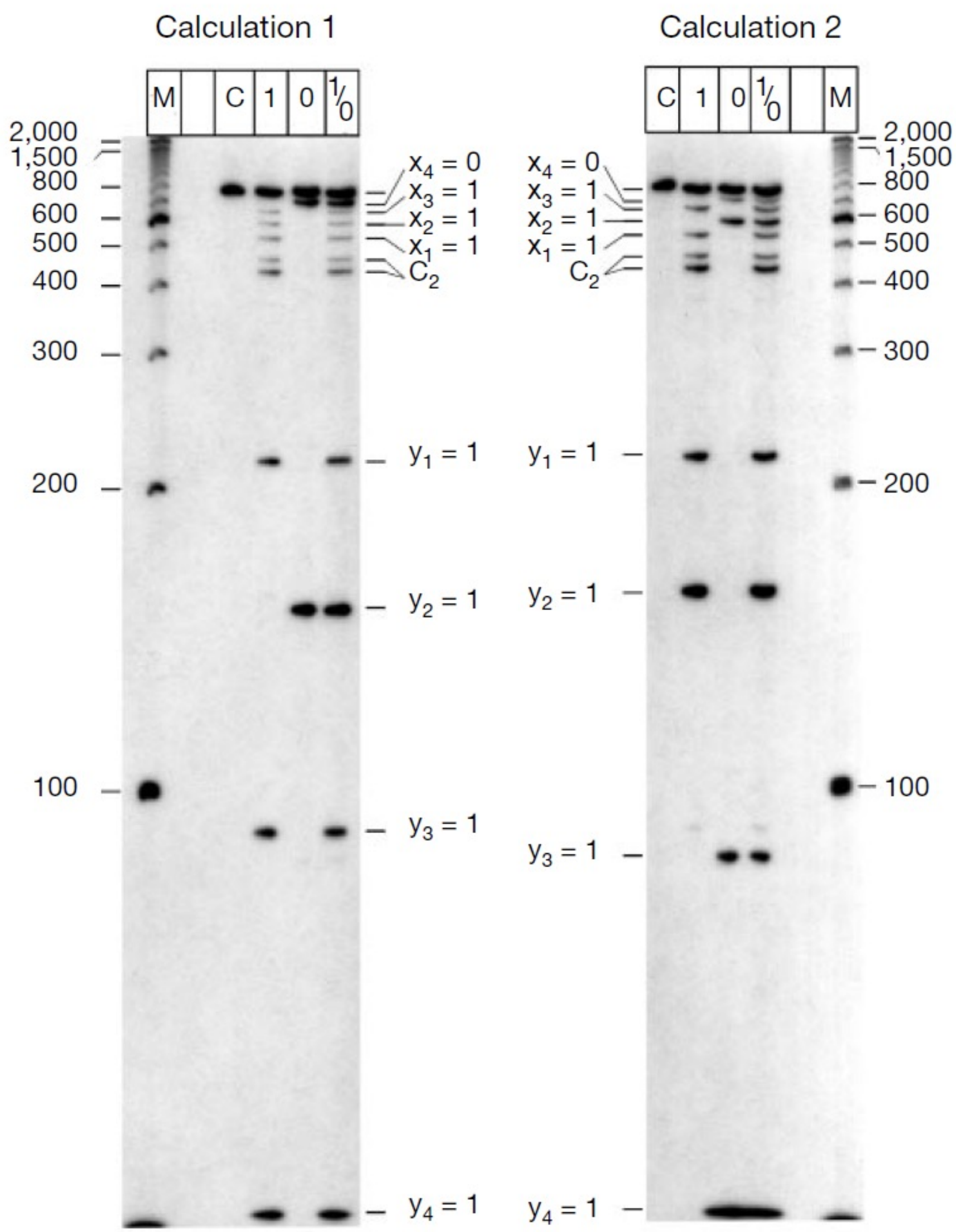
TX Tiles for computing XOR



TX Lattices computing XOR

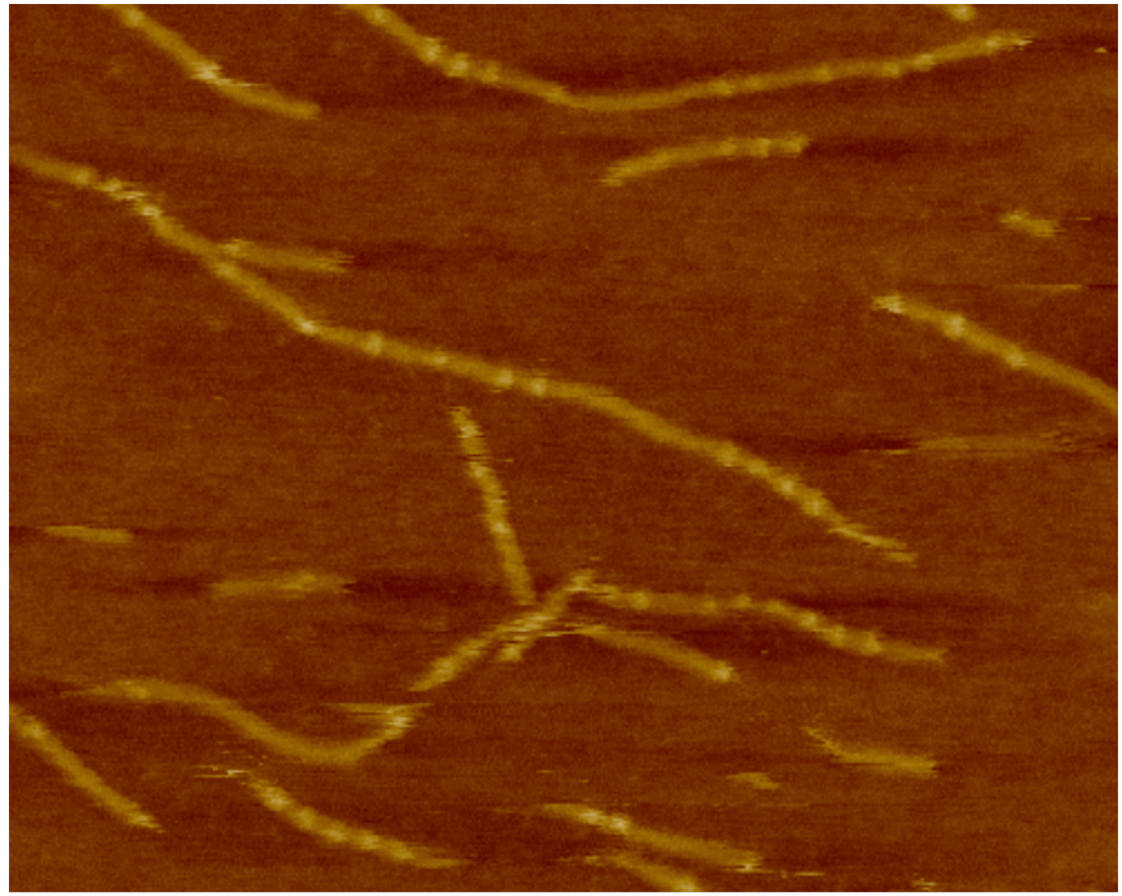
C. Mao, T.H. LaBean, John H. Reif, N. C. Seeman, Logical Computation Using Algorithmic Self-Assembly of DNA Triple-Crossover Molecules, Nature, vol. 407, Sept. 28 2000, pp. 493-495

Gel Electrophoresis Demonstration of Computing using TX tiles



TAE Assemblies for XOR Computation

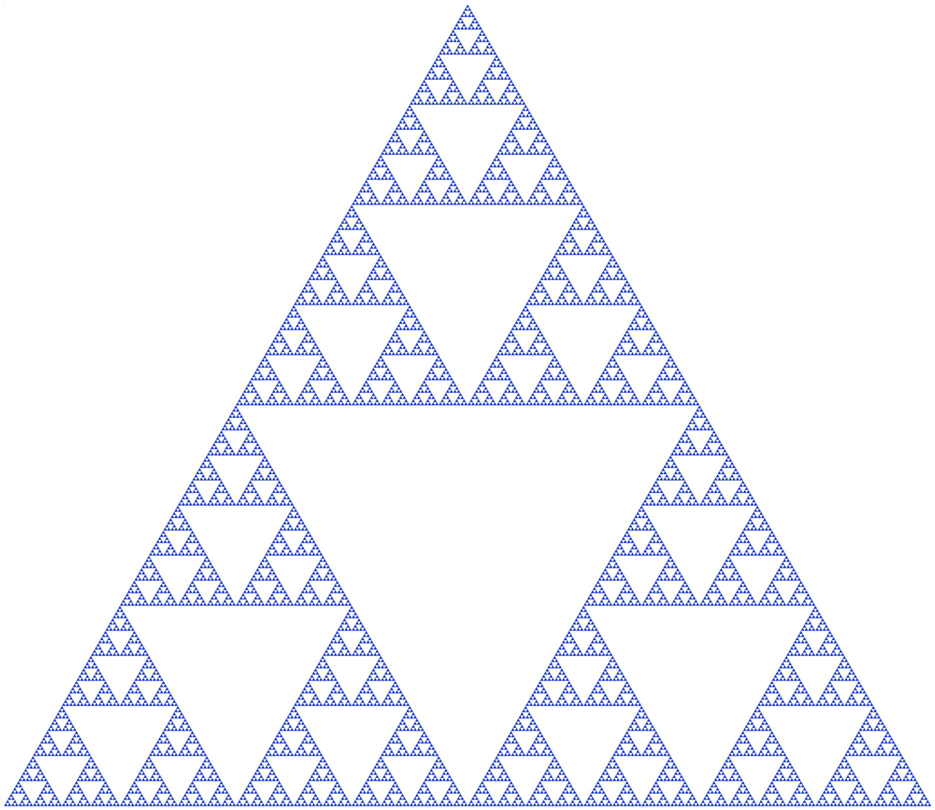
XOR via TAE Computational Complex with Visual Readout



Hao Yan, Liping Feng, Thomas H. LaBean, and John Reif, Parallel Molecular Computations of Pairwise Exclusive-Or (XOR) Using DNA "String Tile" Self-Assembly, JACS (2003).

2D DNA Tiling Computation of a Sierpinski Triangle

Sierpinski Triangle is the Pascal Triangle taken mod 2



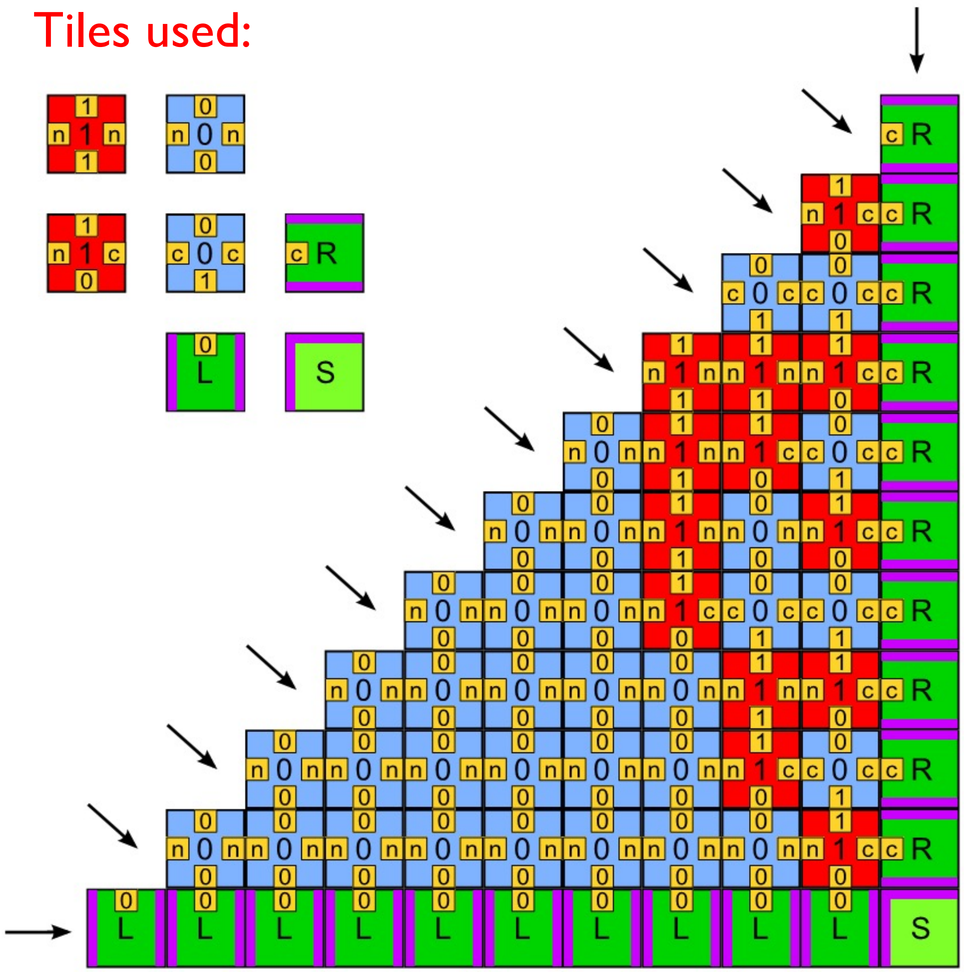
Paul W K Rothemund & Erik Winfree

California Institute of Technology

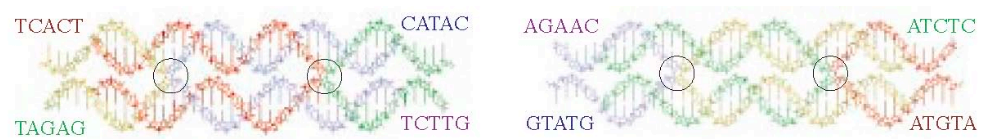
- ***Paul W.K. Rothemund, Nick Papadakis, Erik Winfree, Algorithmic Self-Assembly of DNA Sierpinski Triangles. PLoS Biology (2004)***

Experimental demonstration of Sierpinski Triangle computation via 2D DNA self-assembly:

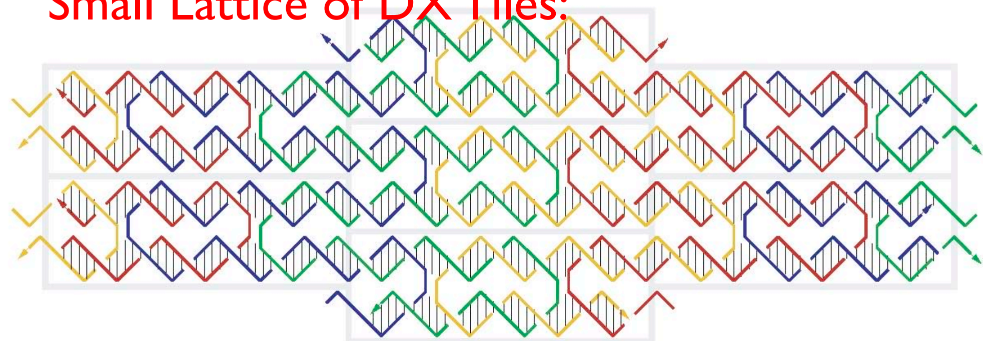
Tiles used:



Used DX Tiles for Computation:



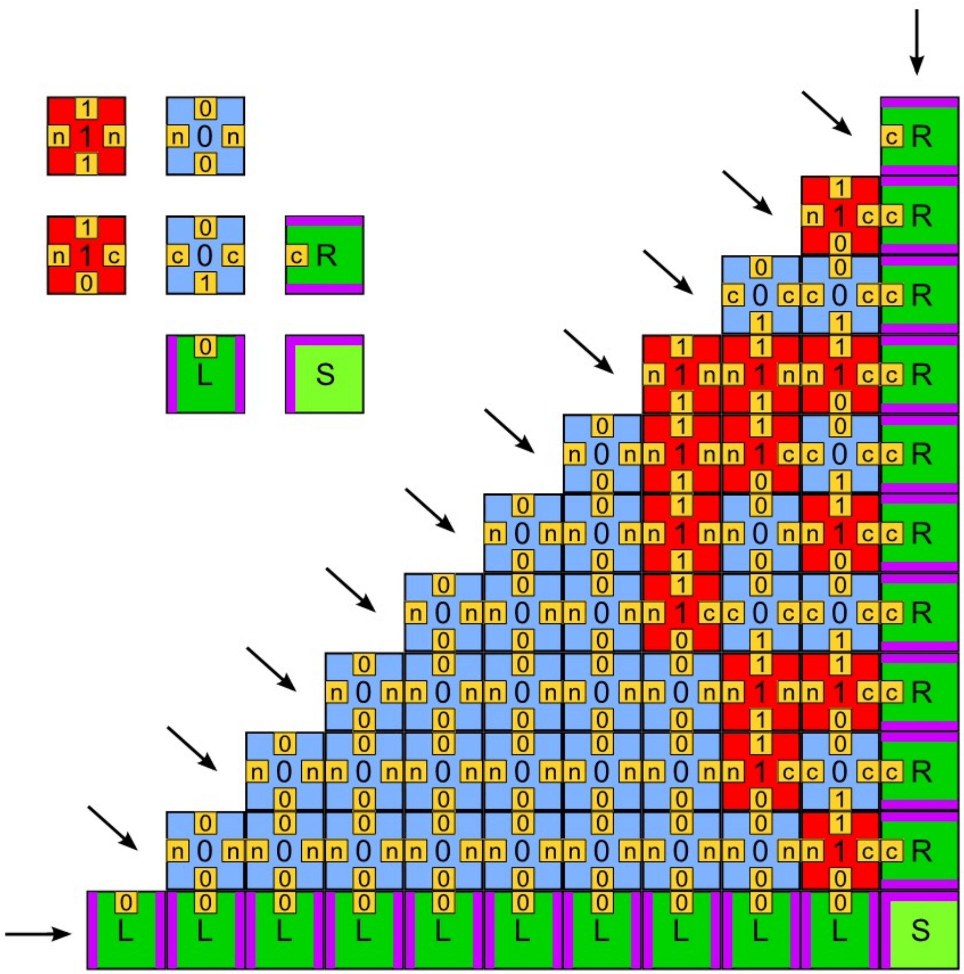
Small Lattice of DX Tiles:

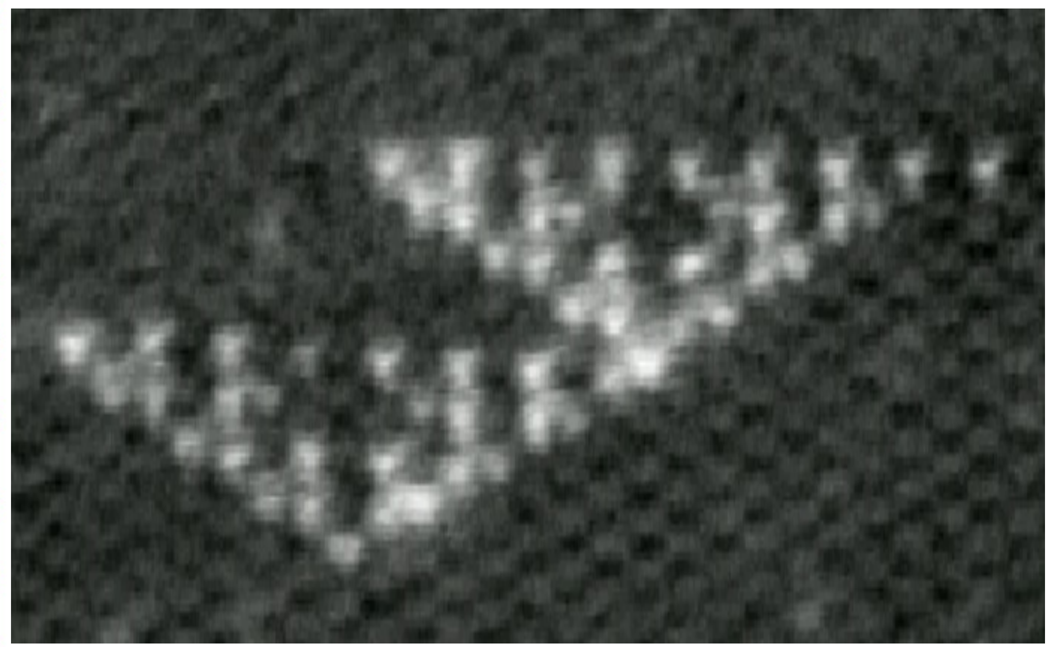


Rothemund, Papadakis, Winfree, Algorithmic Self-assembly Of DNA Sierpinski Triangles

DUKE COMPUTER SCIENCE

Experimental demonstration of Sierpinski Triangle computation via 2D DNA self-assembly:

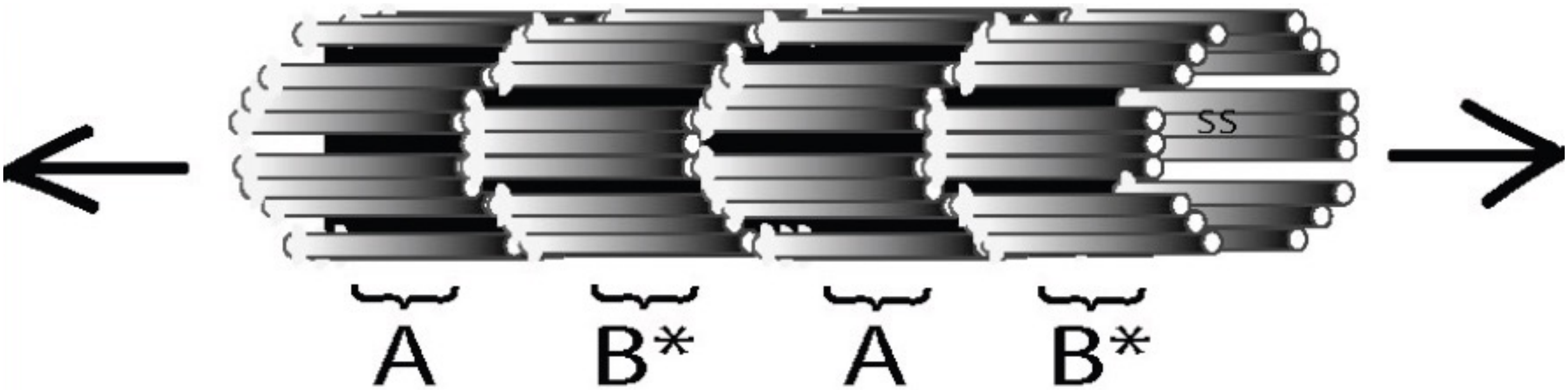




Rothemund, Papadakis, Winfree, Algorithmic Self-assembly Of DNA Sierpinski Triangles

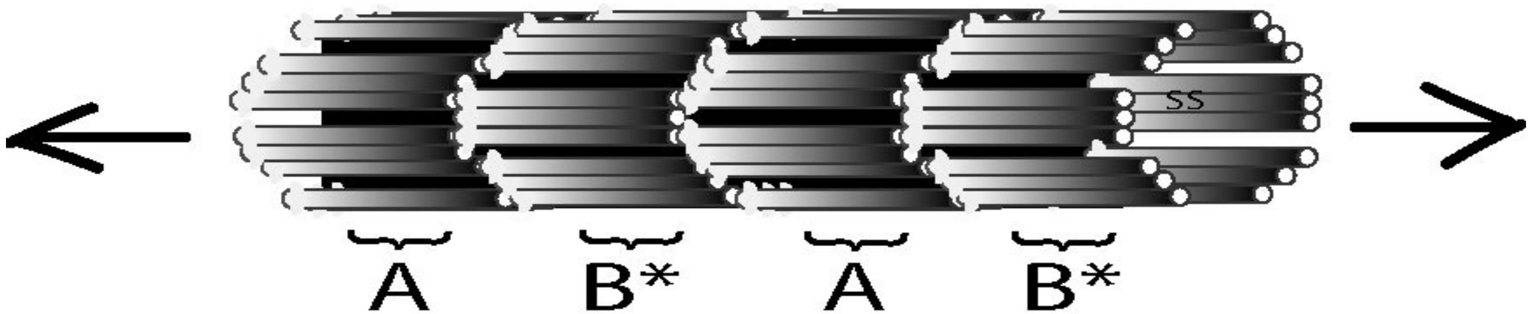
DNA Tubes & Ribbons

TX tubes



Example: Designing C Tile for Nano-Barrel

[redacted]



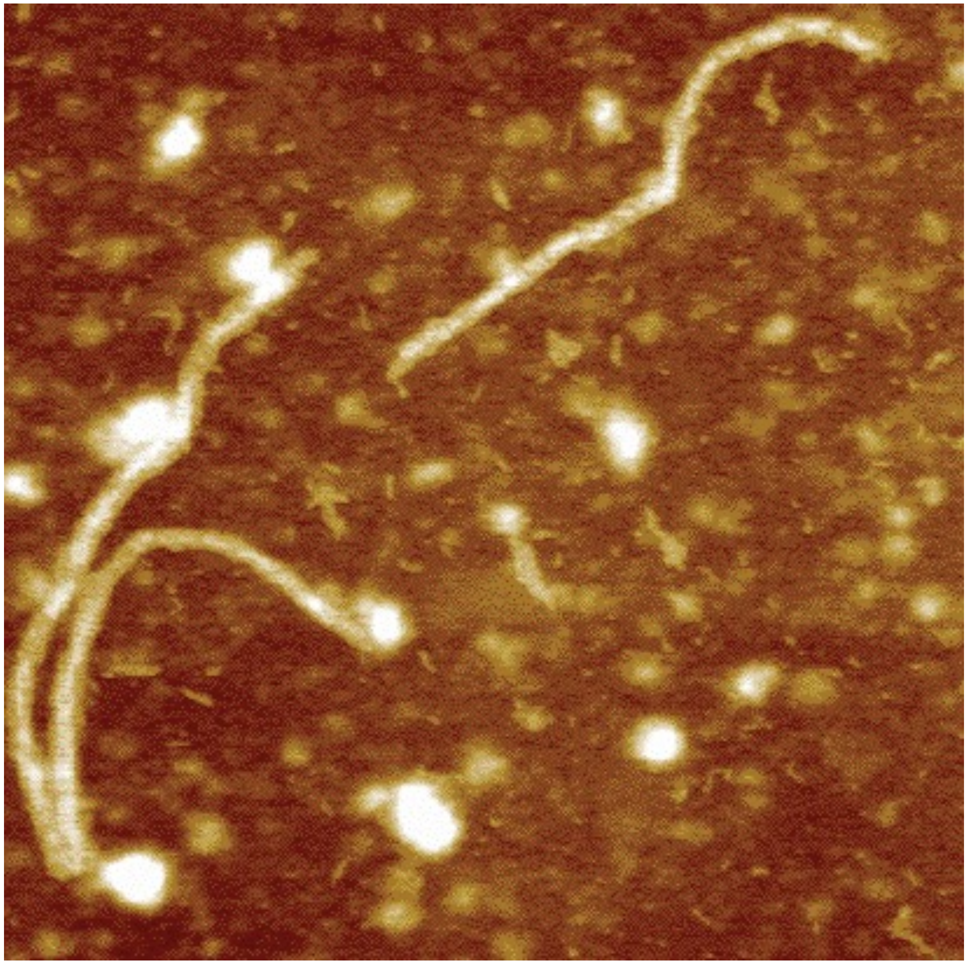
Task: Design C Tile

[redacted]

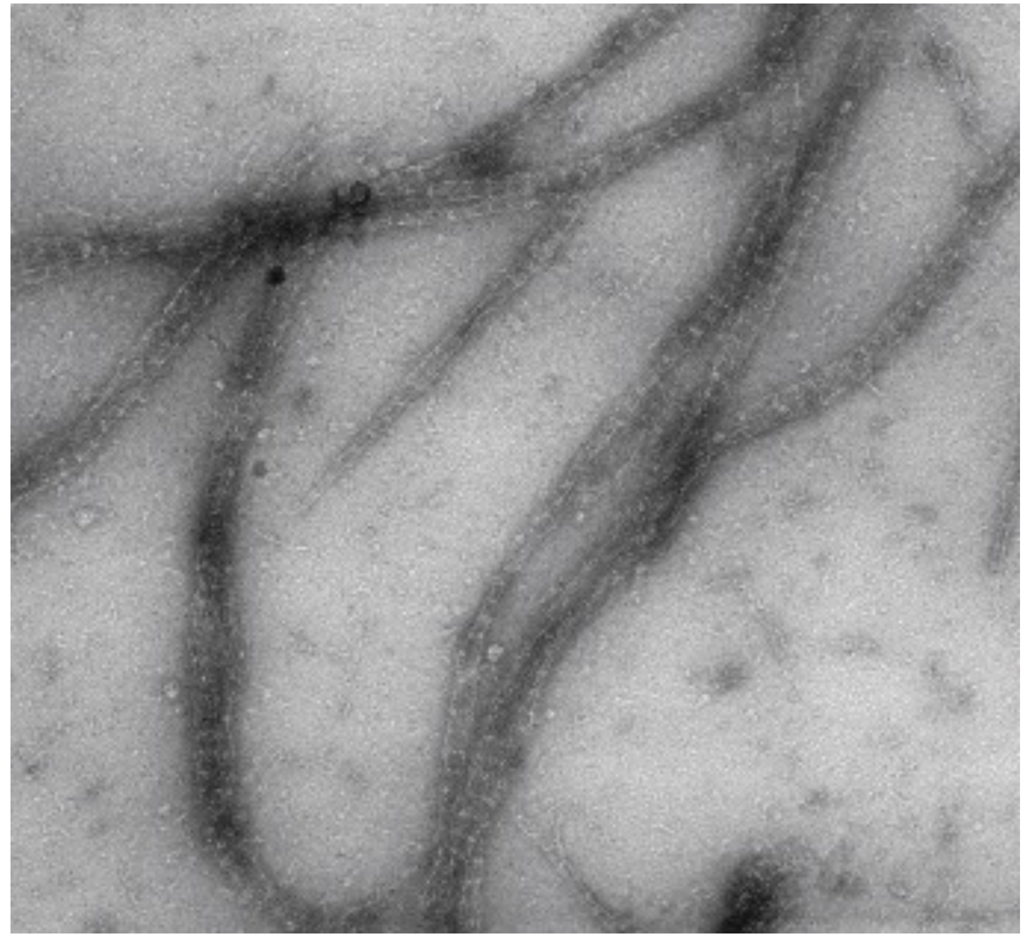
Figure Credit: Thomas. Labean

DUKE COMPUTER SCIENCE

TX tubes



AFM Imaging

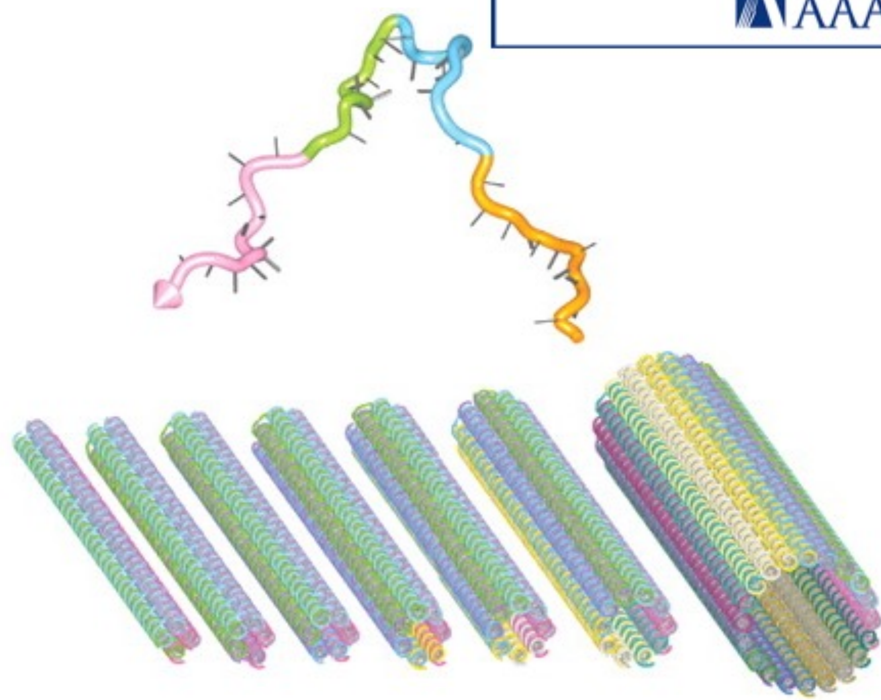


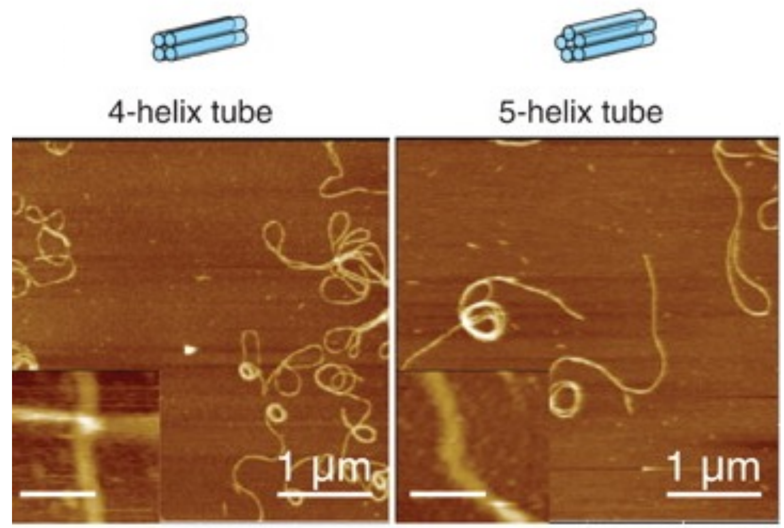
TEM Imaging

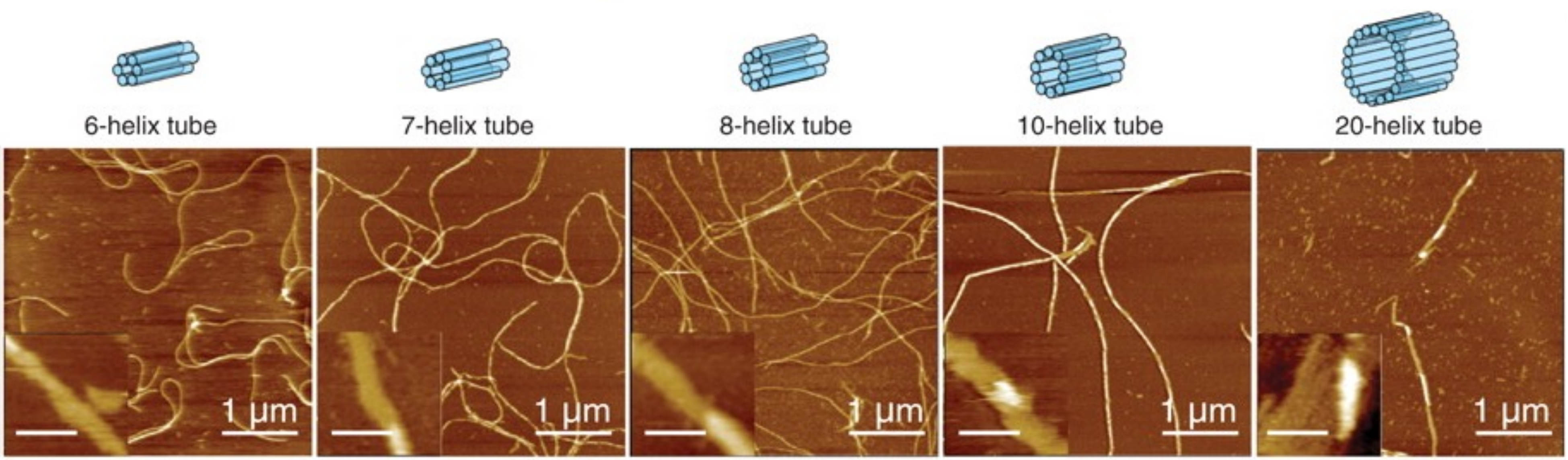
Programming DNA Tube Circumferences

Peng Yin, Reif, et al

Science **321**, 824 (2008);
DOI: 10.1126/science.1157312





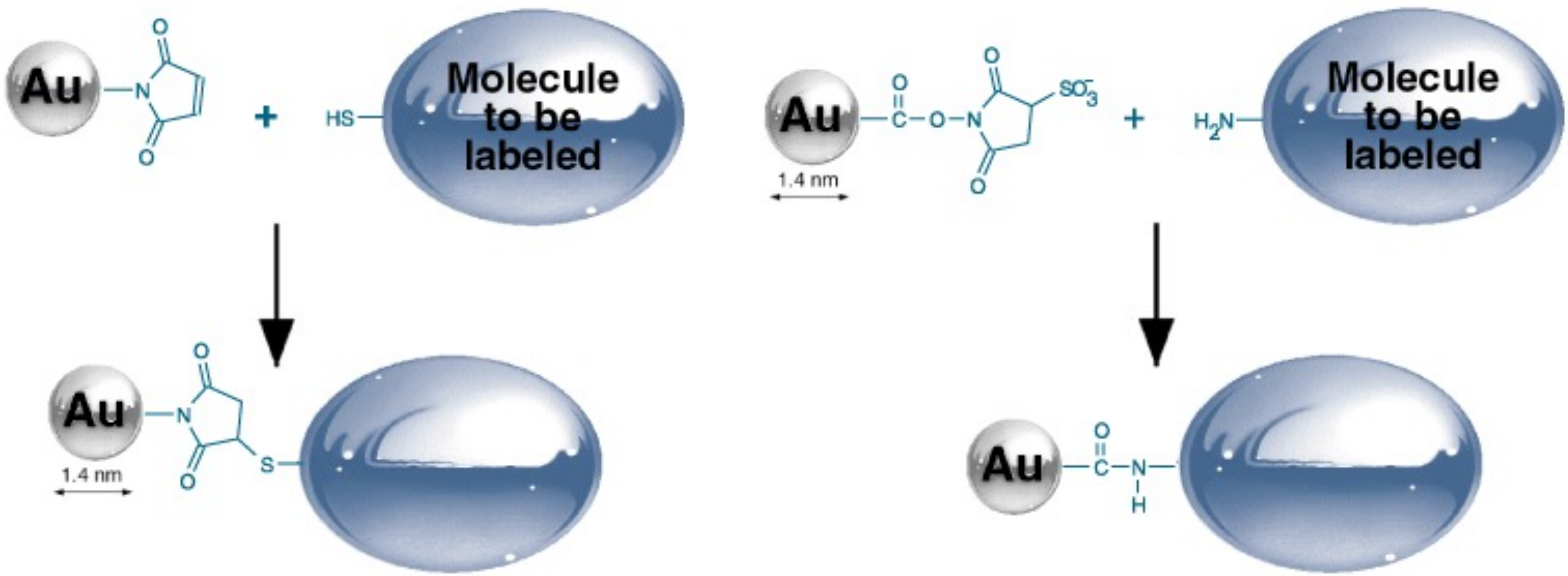


An Application of DNA lattices:

- Molecular Electronics:
  - Layout of molecular electronic circuit components on DNA tiling arrays.

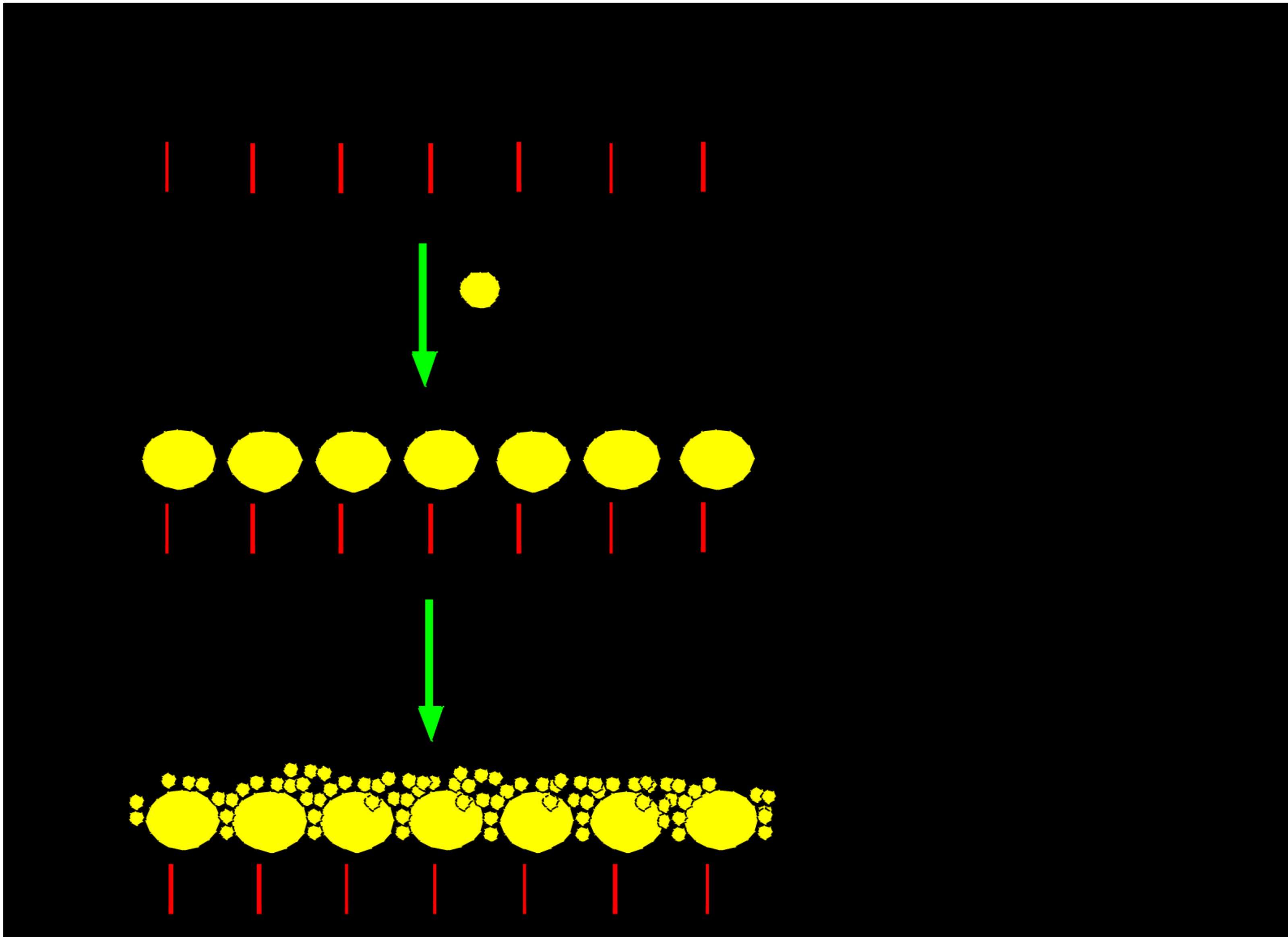
Attachment Chemistries to DNA

- **nanogold + thiol (SH)**
- **nanogold + amino (NH_2)**
- **Other (biotin/avidin, Au/S, etc.)**



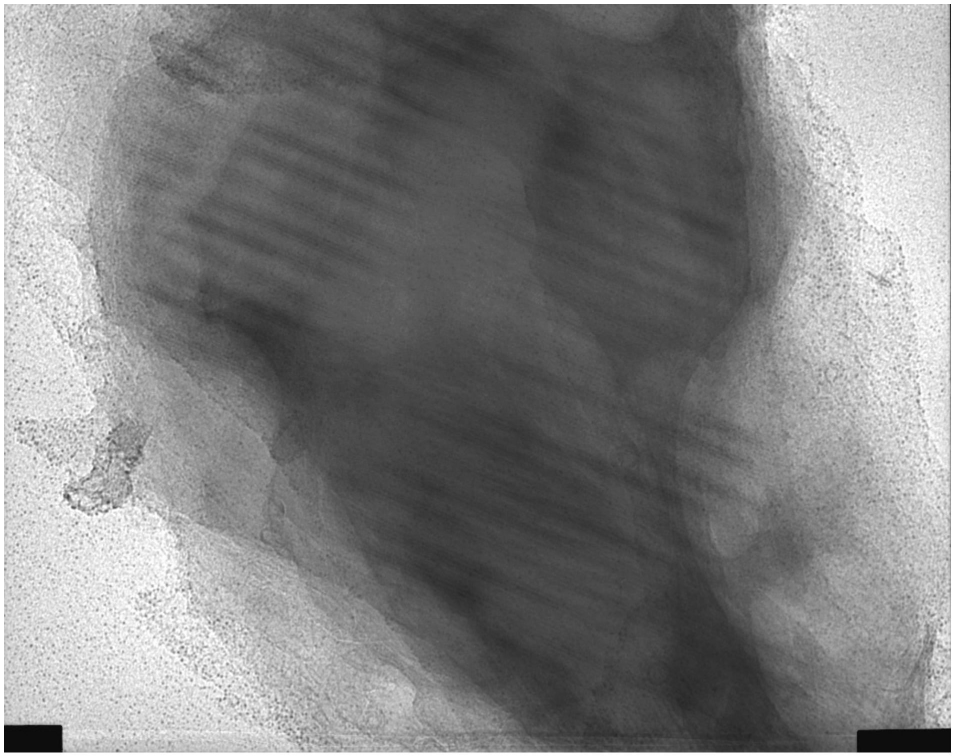
Forming Gold Wires on DNA Tiling Lattices:

- **DNA strands attached to gold beads hybridize at selected tiles of DNA array.**
- **Gold wires forms by fusion of free gold beads to beads attached to DNA array.**
- **Molecular electronics components can self-assemble between the gold breads.**

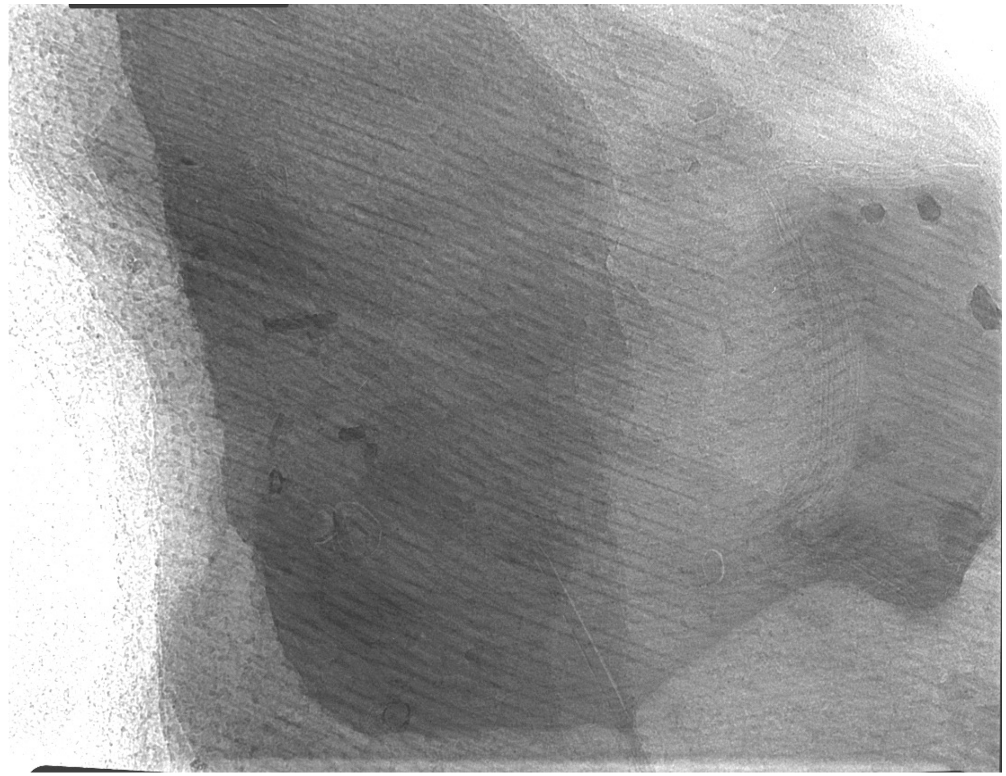


Nanogold Patterning of a DNA Lattice

TEM images of TAO lattices



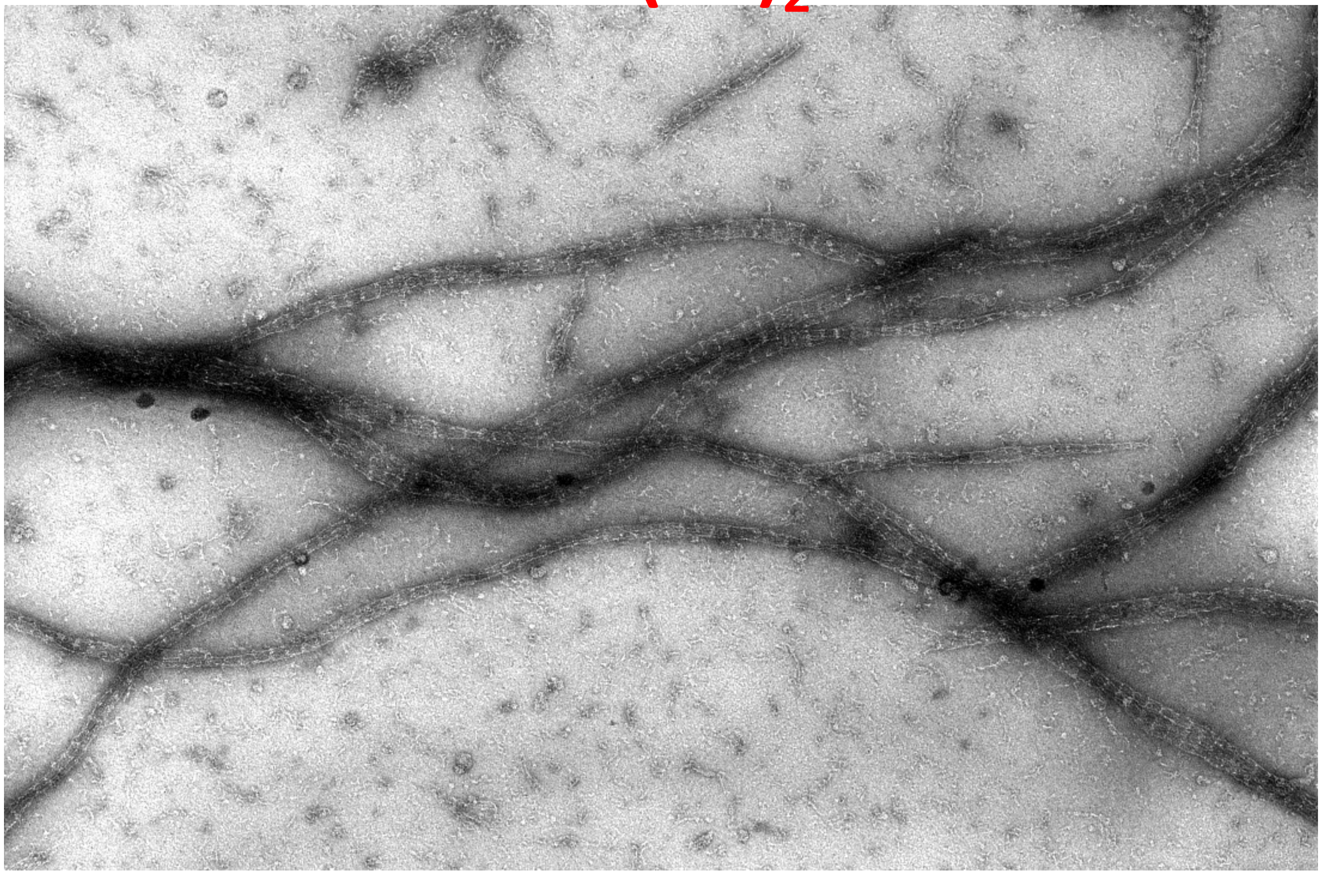
AB* TAO Lattice



ABCD* DX Lattice

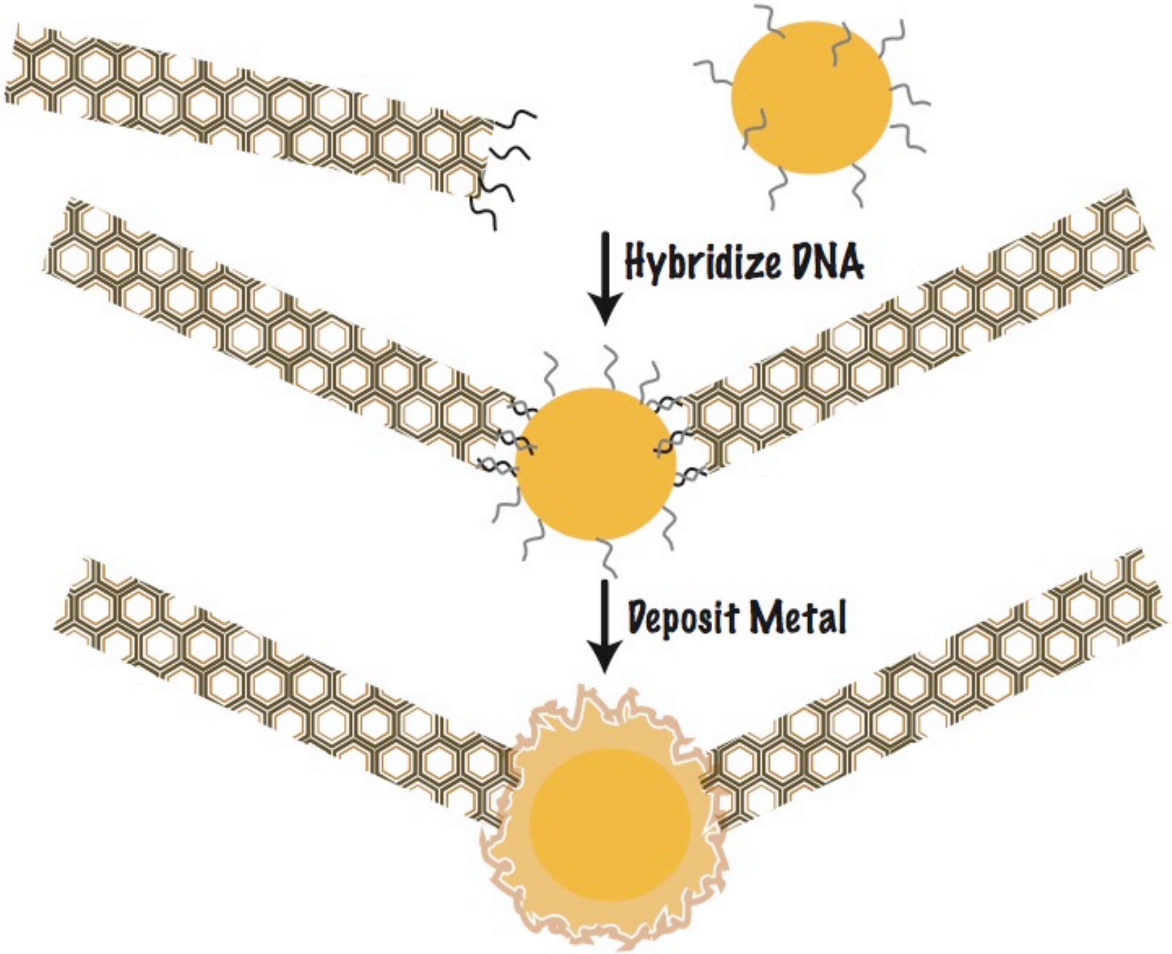
•Moire` interference patterns indicates patterned gold nanoparticles are
•present in multiple layers.
•Electron Diffraction Patterns indicates nanogold is bound in lattice pattern

DNA Fibers from $AB^*(SH)_2$ Tile Lattice



- Self-Assembled DNA Lattices forming fibers of between 5 and 10 microns in length with uniform width (~25 nm) from TAO tiles.
- The fibers result from annealing reactions containing two tile types, A and B*, in which the B* tiles carry a dsDNA stem orthogonal to the tile plane and terminating with a thiol (SH) group on the end of both protruding strands.
- It appears that the thiols associate with other thiols on neighboring tiles and cause a characteristic curling of the lattice resulting in formation of tubes instead of sheets.
- An addition dsDNA stem protruding from the "underside" of B* tiles produces the stripes visible on the outside of the tubes.

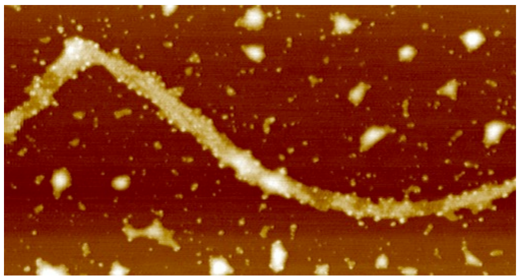
Using DNA for Targeted Conductive Nanowire Connections



Lebeck & Sorin, Duke,New Directions in Computer Architecture enabled by DNA NanoTech

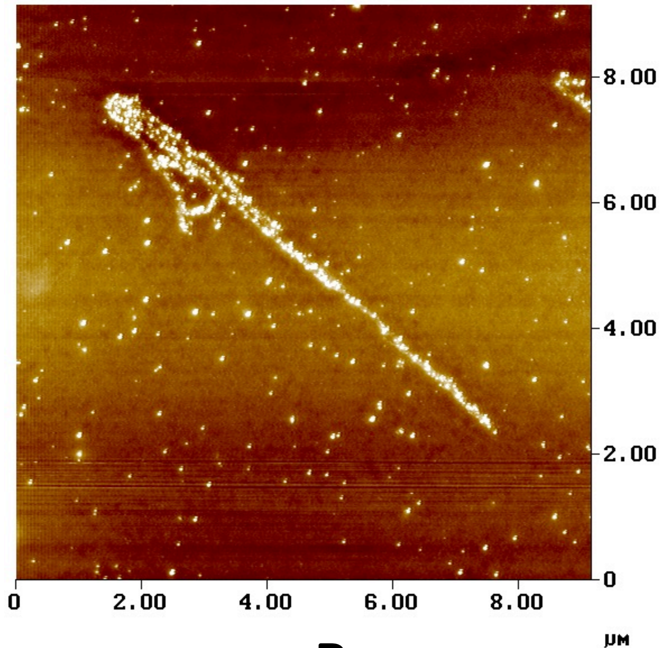
Targeted Metallization of AB* Fibers:

AFM images of progressive metallization of AB*$(SH)_2(NH_2)$ Fibers.



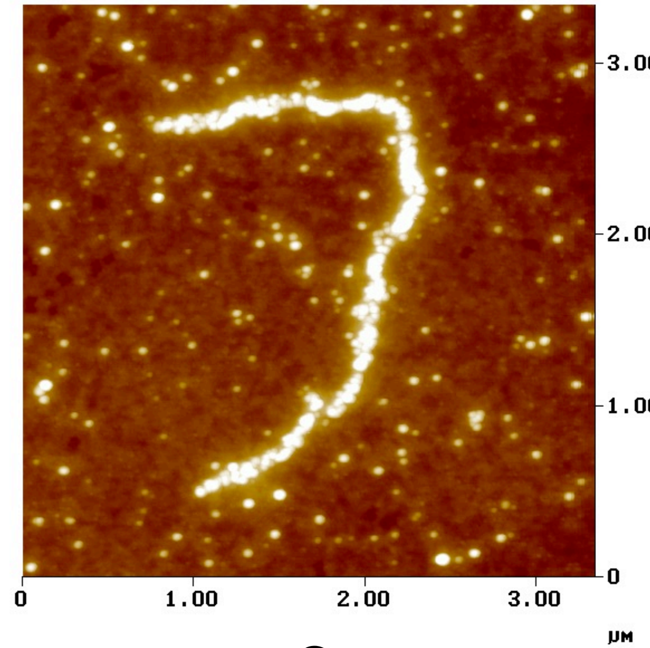
A

Monofunctional nanogold (1.4 nm) bound to NH_2 groups on surface of fibers.



B

Silver Enhanced staining deposited silver on the bound gold (2 minutes).



C

Silver Enhance staining (5 minutes). Note nearly continuous metal wire.

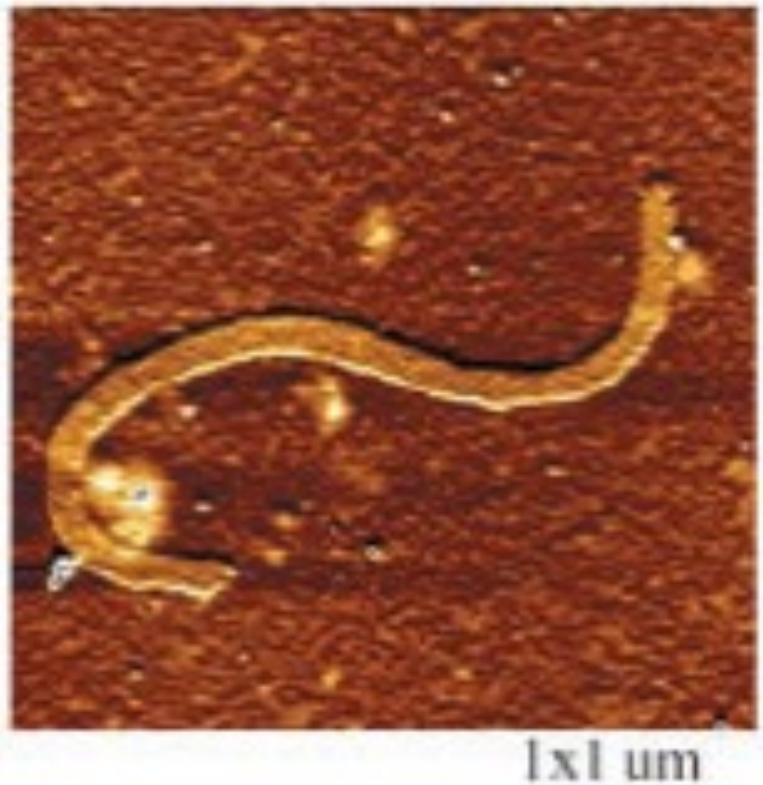
Procedure of Electrical Measurement of DNA-Based Metallized Nanotubes

Process of experimental Setup for measuring conductivity of DNA-based devices

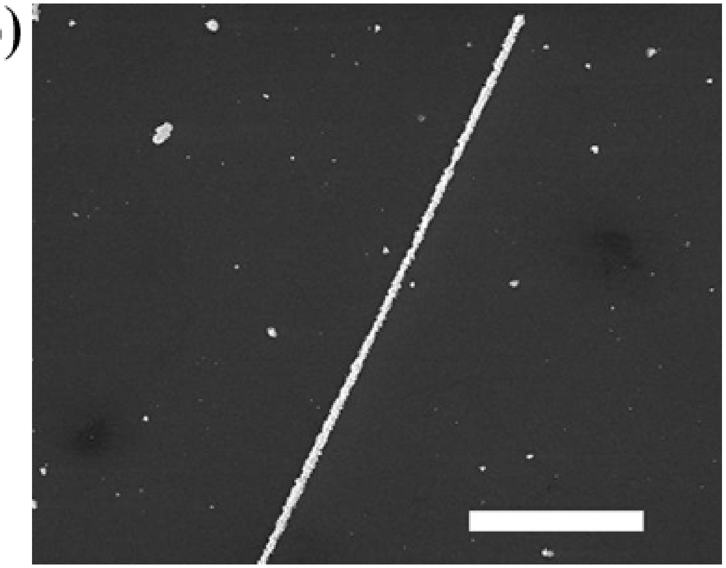
- **Compact electronic circuit may be possible using nanometer-scale DNA nanotubes**
- **Position controllable using carefully designed DNA bases**

Silver (Au) Metallization of 4x4 DNA Lattice ribbon and Conductivity Measurement

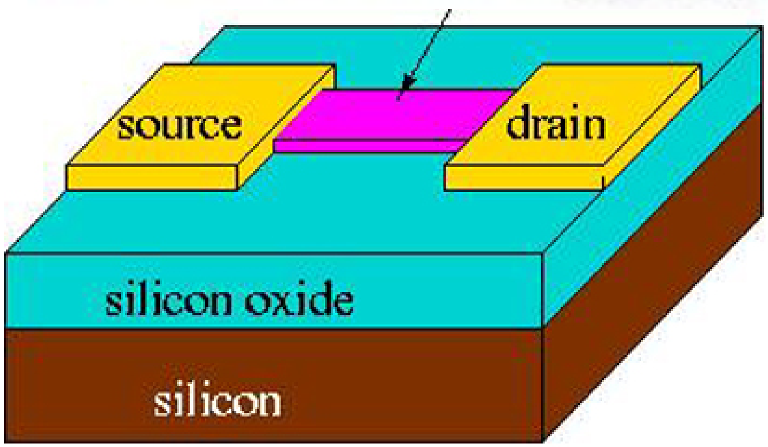
a)

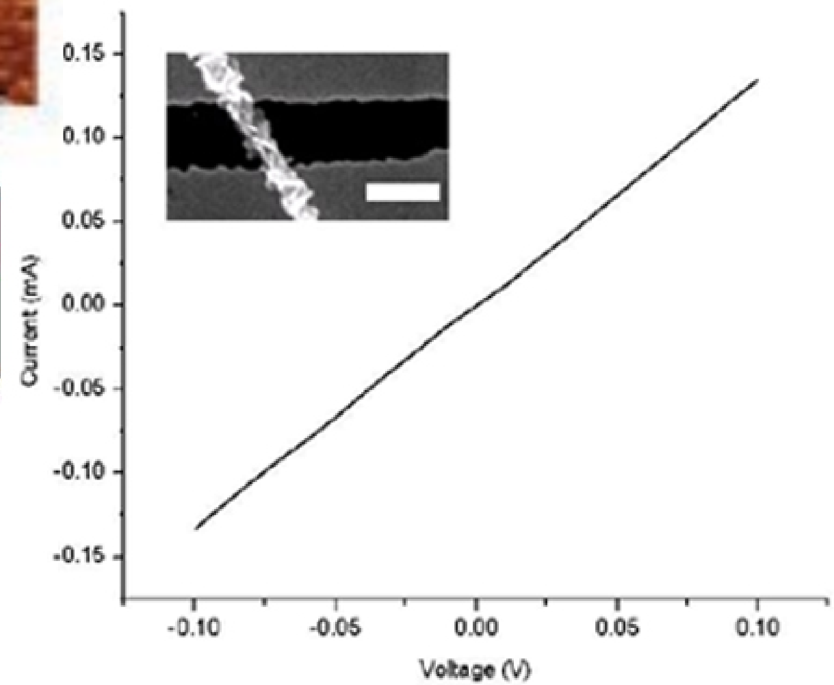


b)



c)

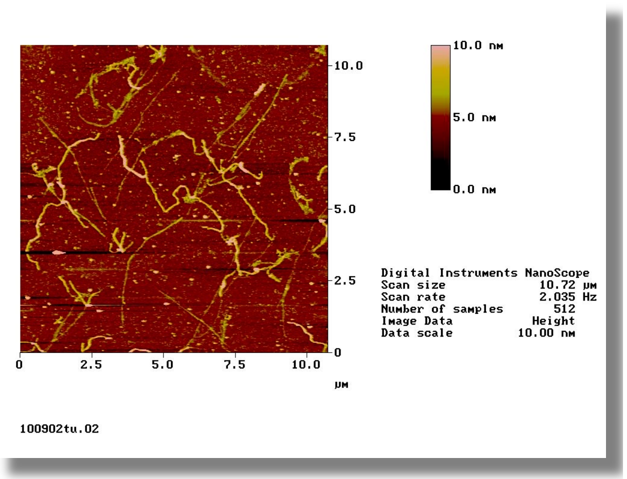




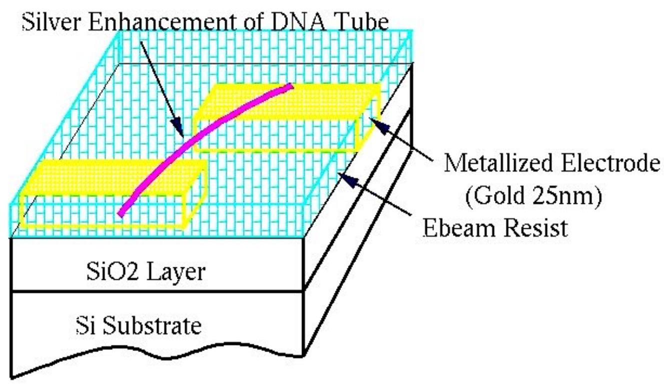
Hao Yan, Sung Ha Park, Liping Feng, John Reif, and Thomas H. LaBean, Science (2003)

Two Processes of Conductivity Measurement for Metallized DNA Nanotubes

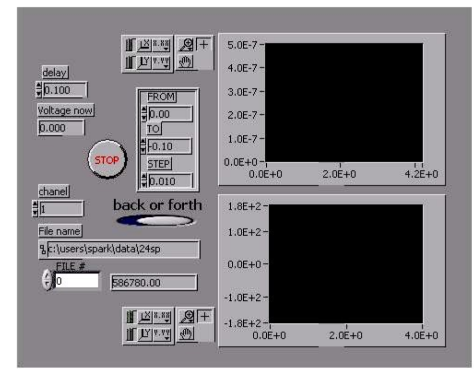
Random Deposition Nanotubes with Electron Beam Lithography process



(a)



(b)

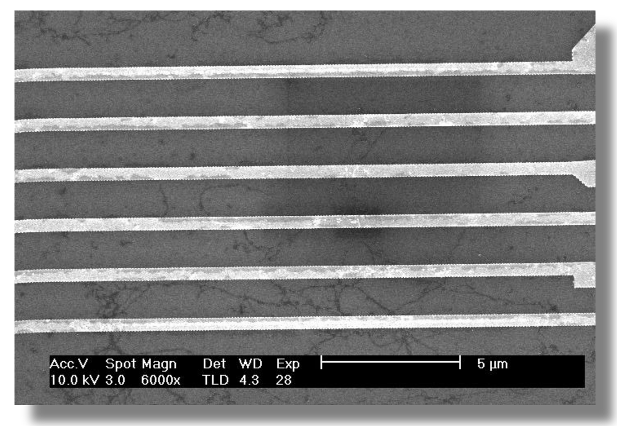


(c)

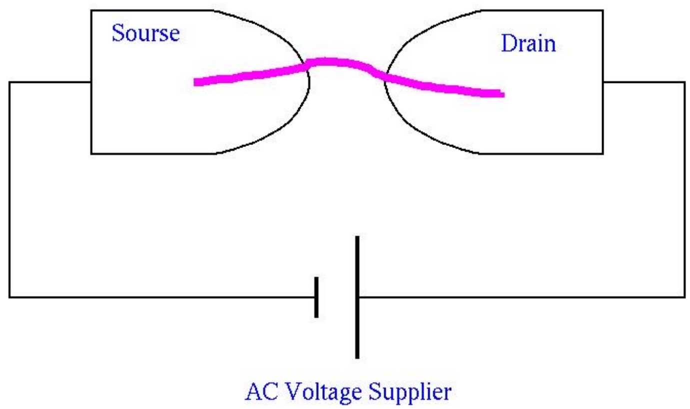
(a) Preparation Metallized DNA Tubes on Silicon Substrate

(b) Electron Beam Patterning

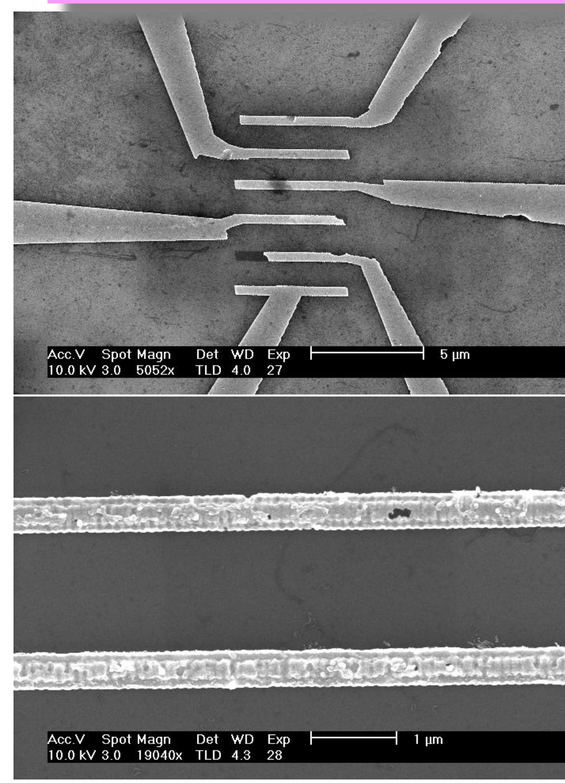
(c) Electric Measurement using LabView Interface



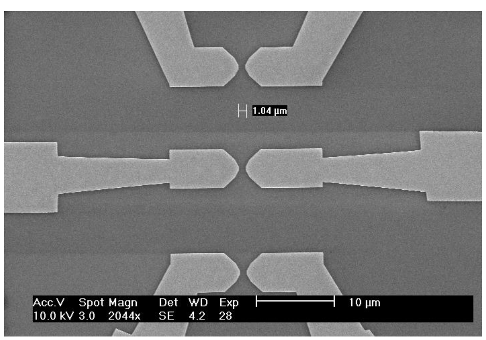
Trapping DNA Nanotubes using AC Voltage



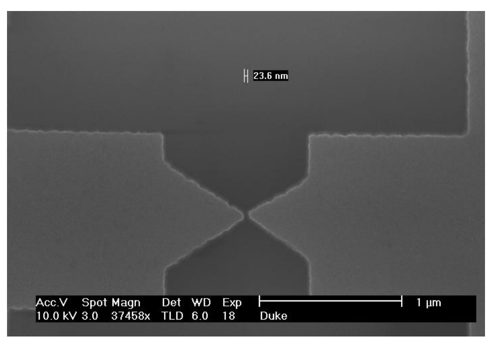
(c) After Trapped Tubes



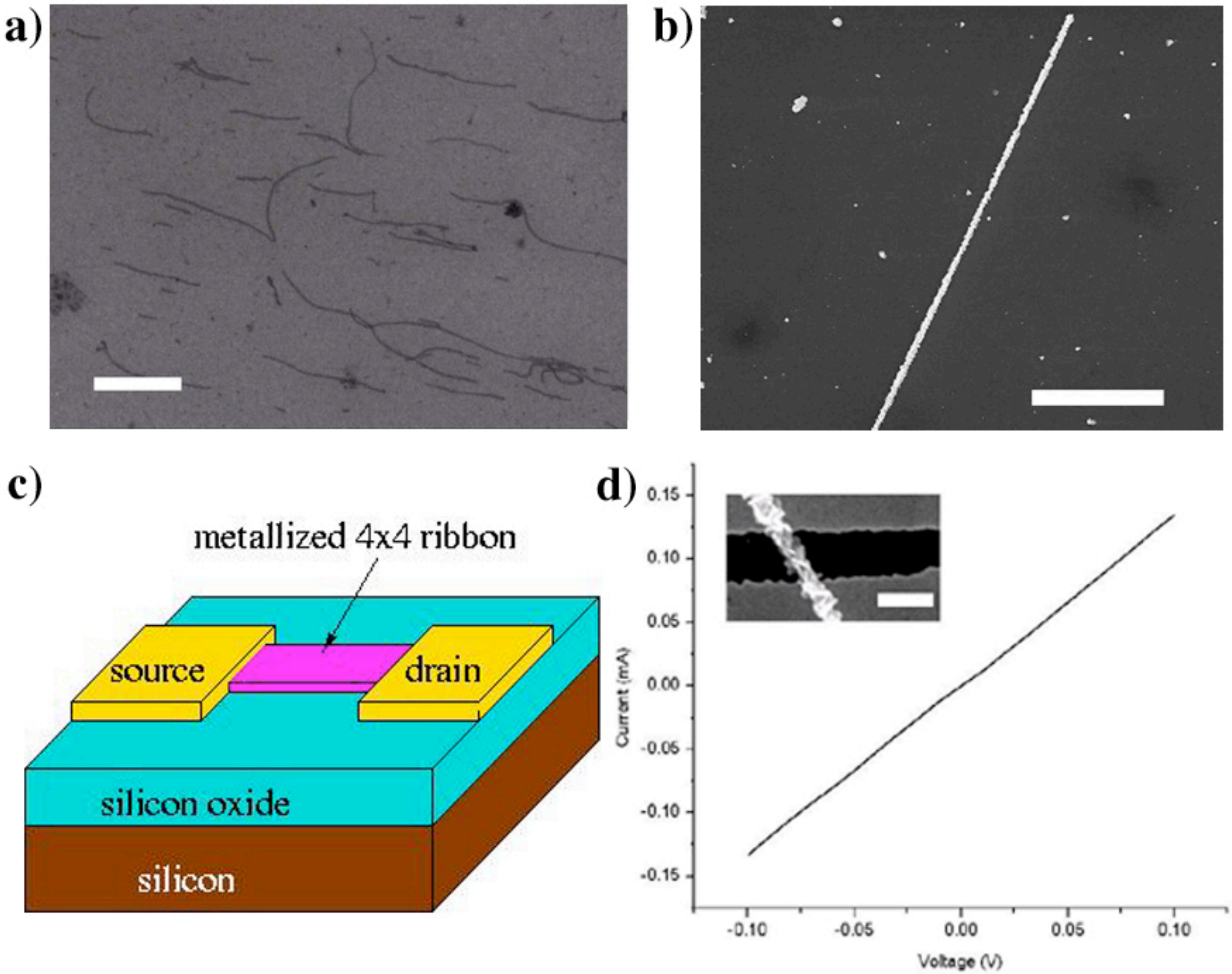
(a) Preparation of Metal Electrodes



(b) Trapping Tubes ; Apply AC Voltages (e.g., 1V, 50kH, 30sec)



2-Step procedure Au Metallization of 4x4 ribbon and Conductivity Measurement



Patterned DNA Lattices

Directed Nucleation Assembly:

A method for assembly of complex patterns

- Use artificially synthesized DNA strands that specify the pattern and around which 2D DNA tiles assemble into the specified pattern.
- The permanent features of the 2D pattern are generated uniquely for each case.

Directed Nucleation Self Assembly Steps:

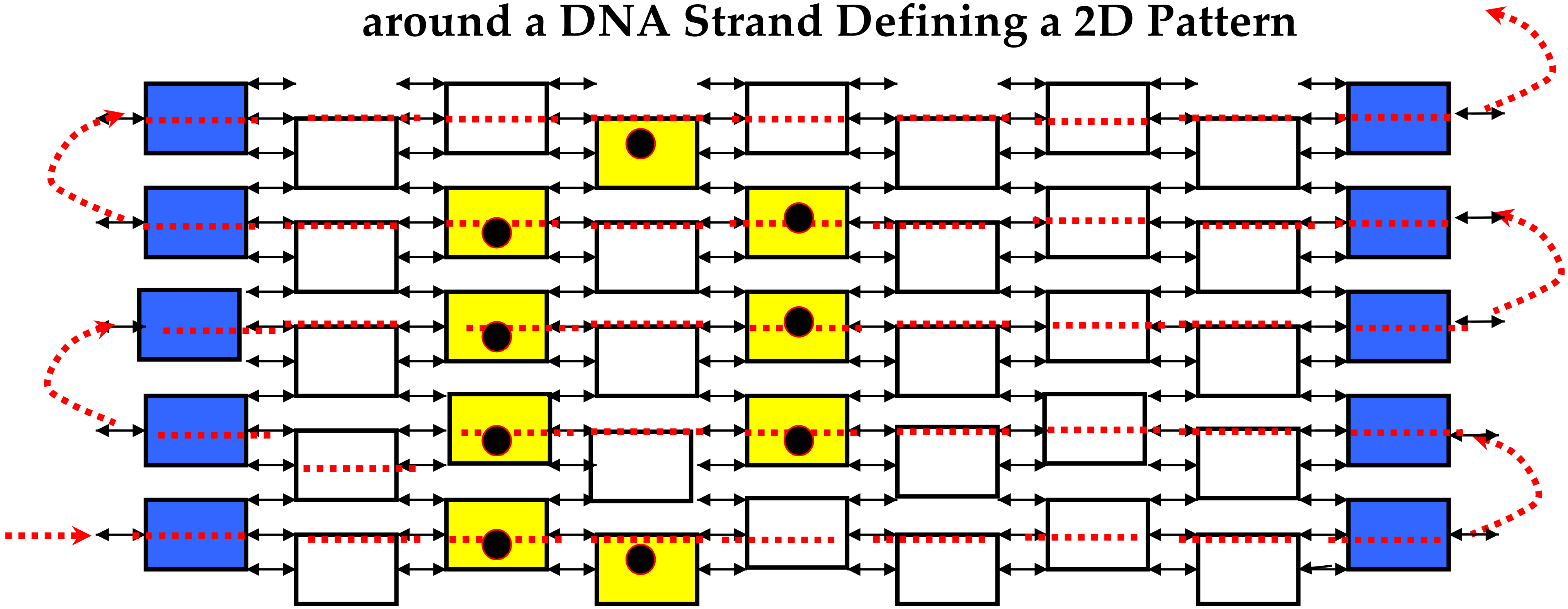
- an input DNA strand is synthesized that encodes the required pattern
- then specified tiles assemble around blocks of this input DNA strand, forming the required 1D or 2D pattern of tiles.

2D DNA Self-Assembled Tiling

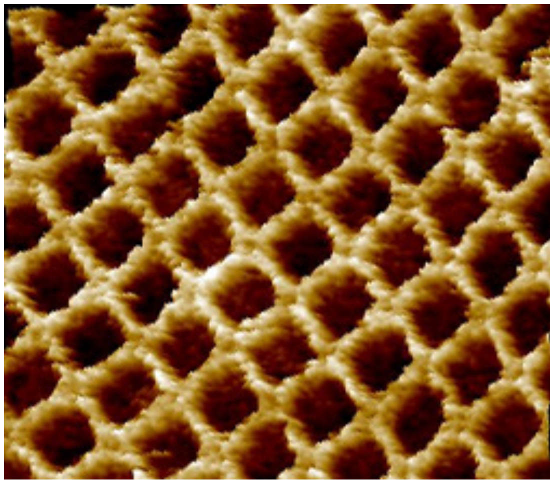
The Process of Assembling a 2 D Pattern by Directed Nucleation :

Self Assembly of Tiles

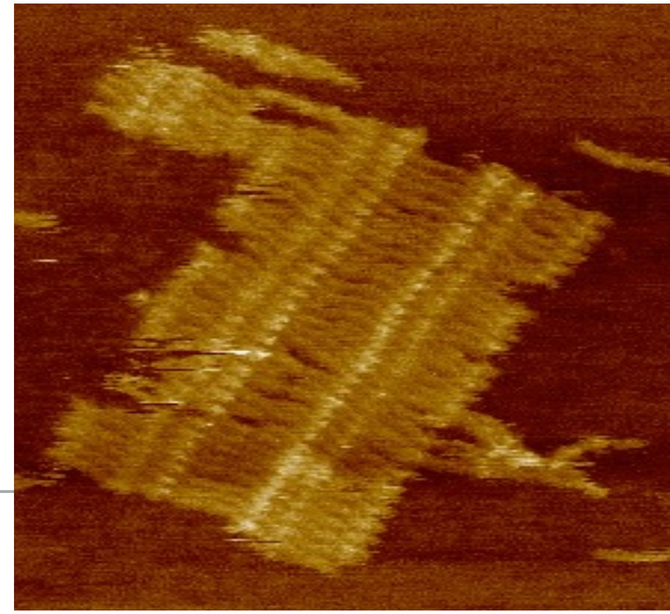
around a DNA Strand Defining a 2D Pattern



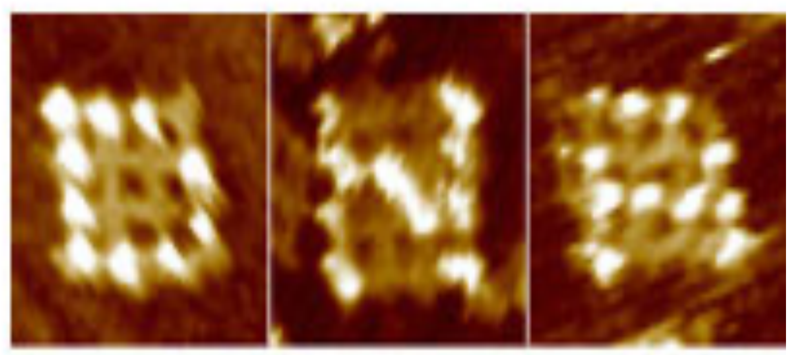
Programmable Patterned DNA Nanostructures



NOT Patterned

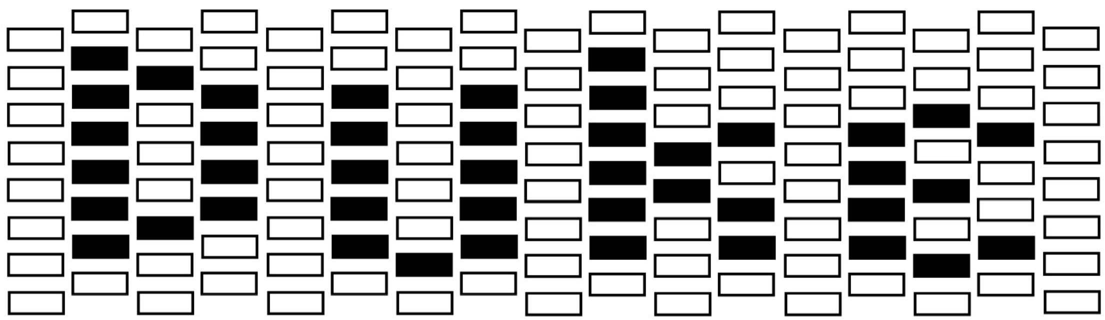


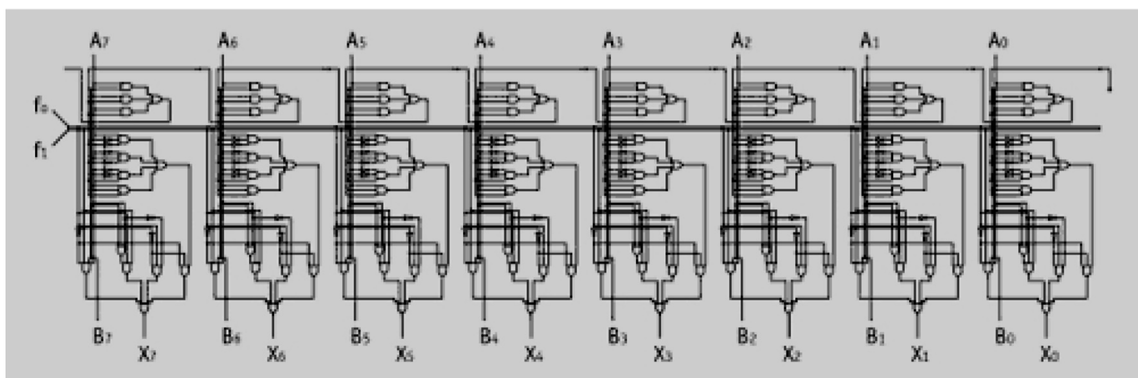
Patterned



Patterned DNA lattices:

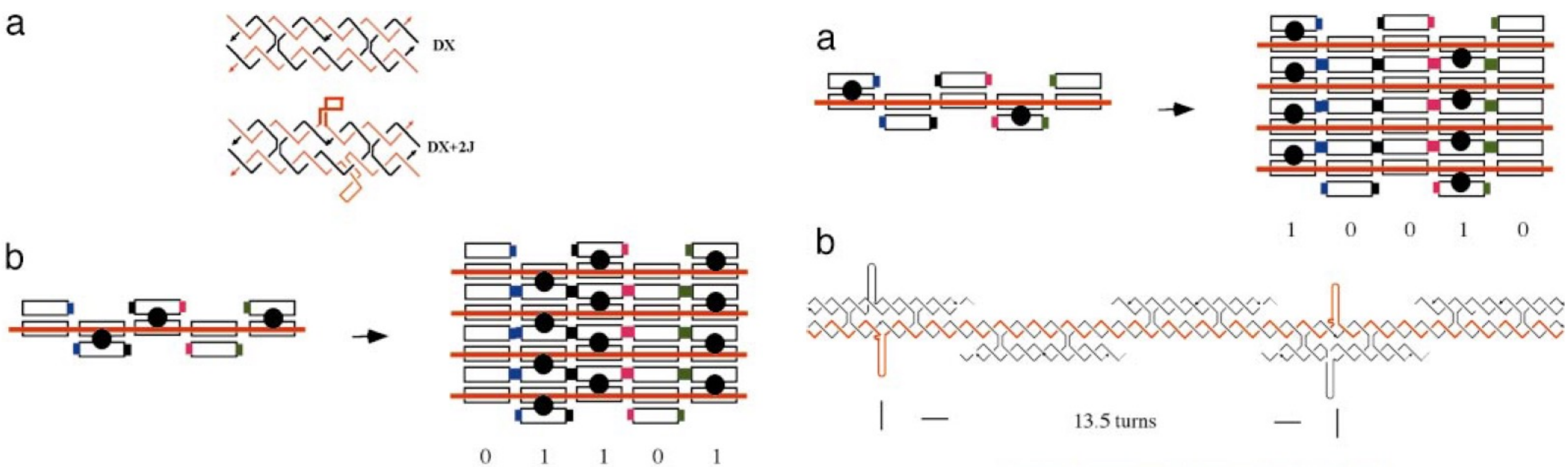
- **Allows for Attachment of Nanoparticles at Specific Sites on Lattice**





- **Application: Molecular Electronics:**
  - **Layout of molecular electronic circuit components on DNA tiling arrays.**

Barcoded lattices



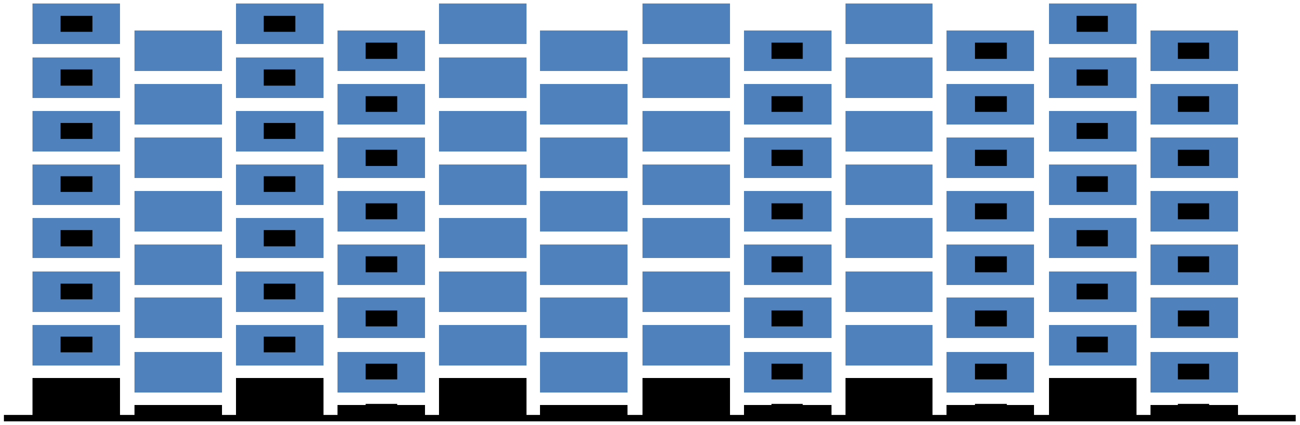
Hao Yan, Thomas H. LaBean, Liping Feng, and John H. Reif, Directed Nucleation Assembly of Barcode Patterned DNA Lattices, Proceedings of the National Academy of Science(PNAS), Volume 100, No. 14, pp. 8103-8108, July 8, (2003)

Molecular Pattern Formation using Scaffold Strands for Directed Nucleation: *H Yan, T LaBean, L Feng, J. Reif, PNAS (2003).*

- Multiple tiles of an input layer can be assembled around a single, long DNA strand we refer to as a scaffold strand (shown as black lines in the figures).

Hao Yan

Barcode lattice displays banding patterns dictated by the sequence of bit values programmed on the input layer:

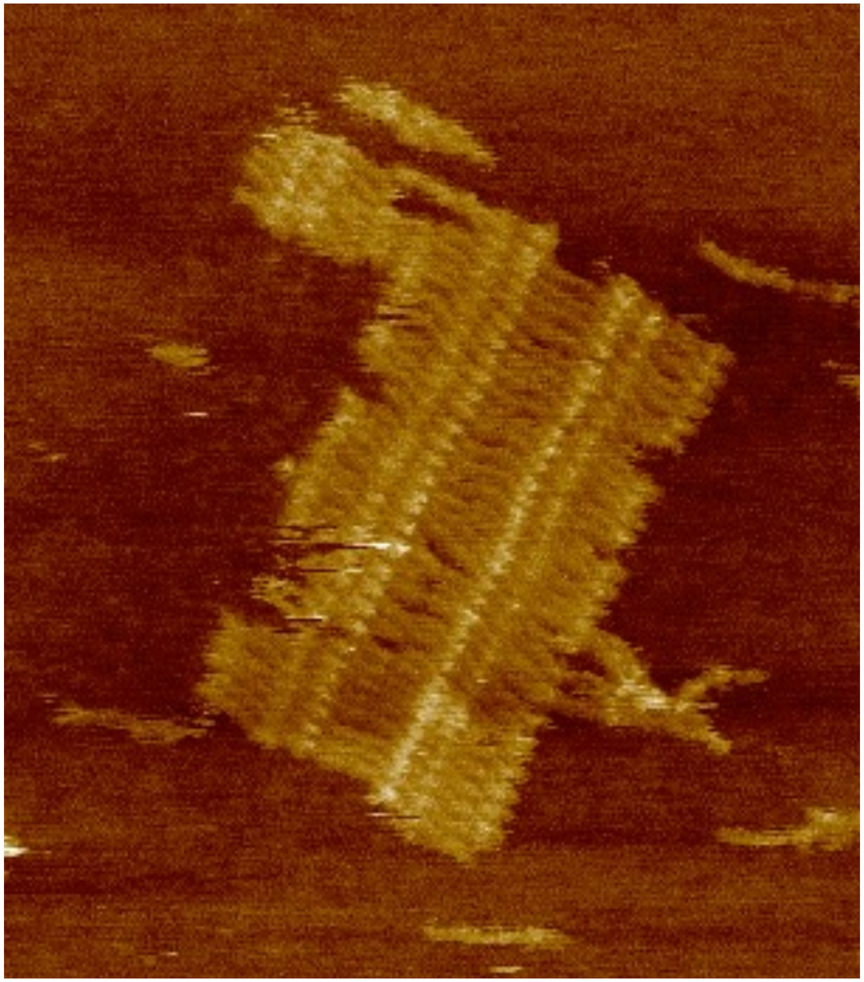


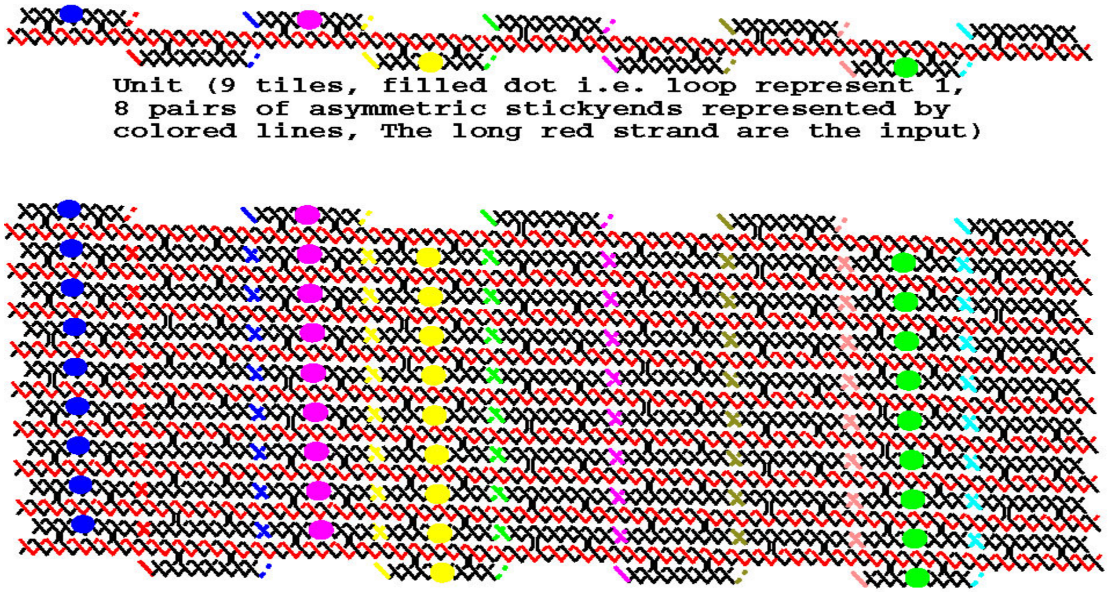
- **Extends 2D arrays into simple aperiodic patterning:**
  - The pattern of 1s and 0s is propagated up the growing tile array.
  - The 1-tiles are decorated with a DNA stem-loop pointing out of the tile plane (black rectangle) and 0-tiles are not.
  - Columns of loop-tiles and loopless-tiles can be distinguished by AFM as demonstrated with periodic AB* lattice.

Barcode Lattice for Rendering 1 D Patterns:

H Yan, T LaBean, L Feng, J. Reif, PNAS (2003).

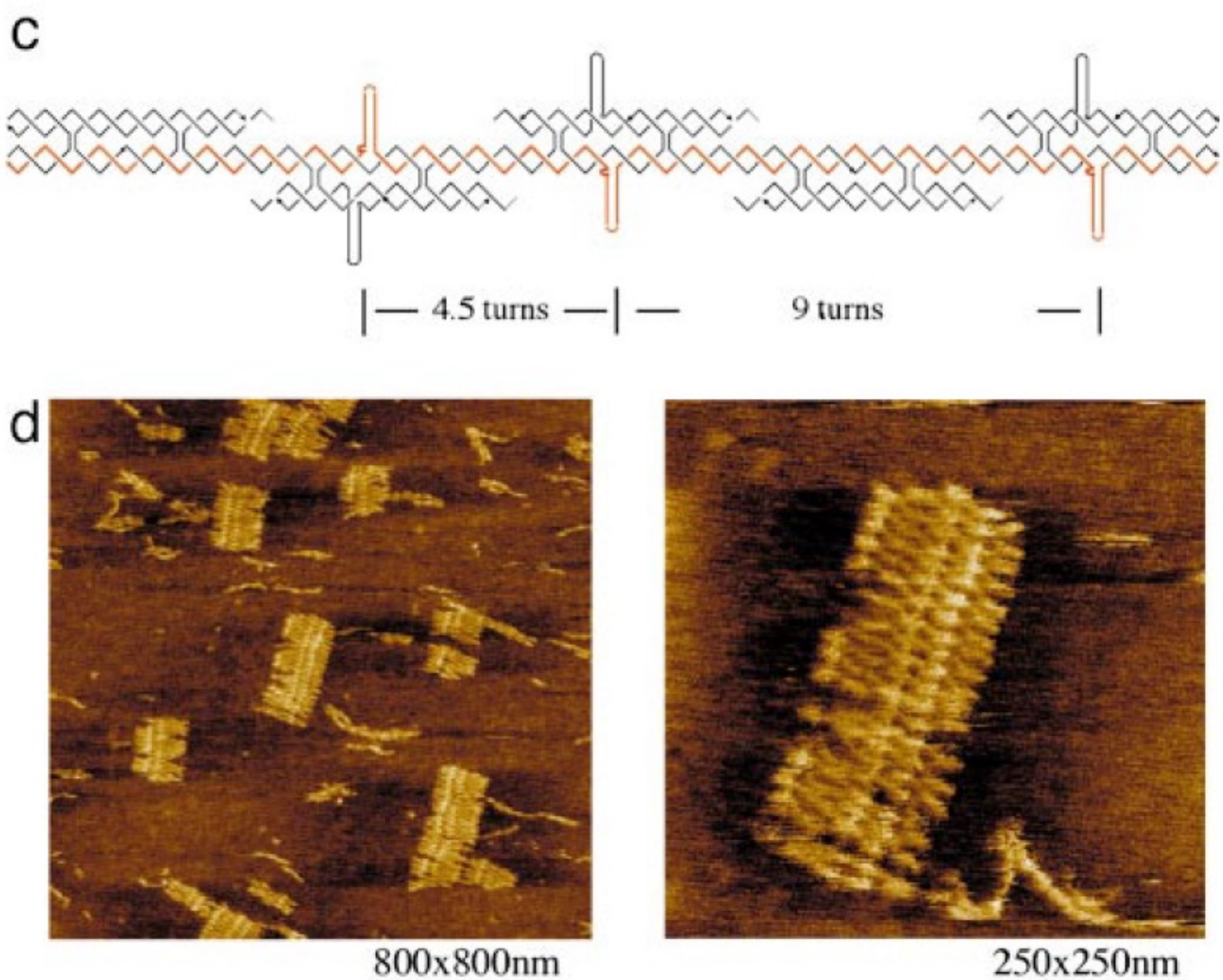
Hao Yan





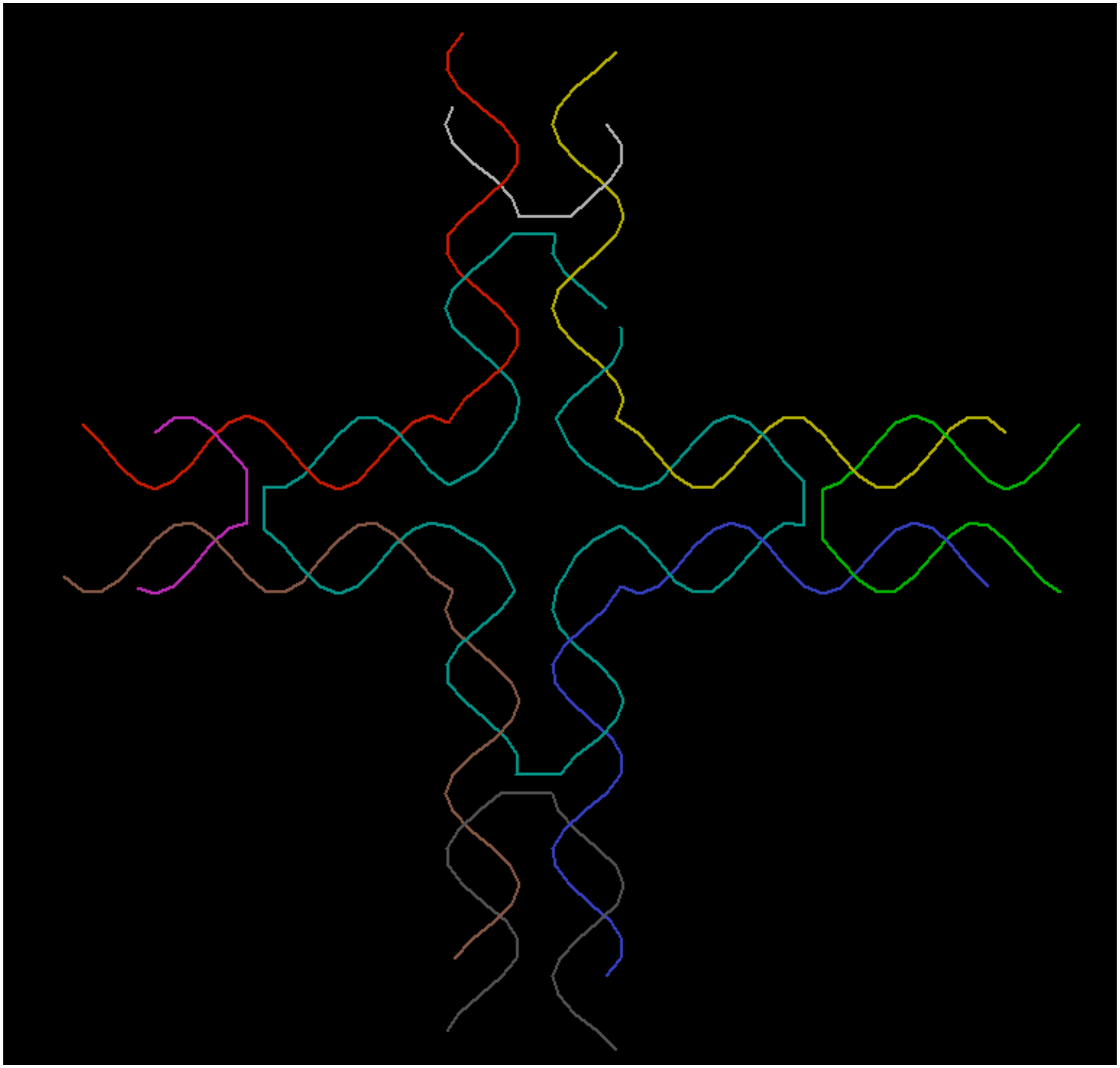
Barcode lattice displays banding patterns dictated by the same sequence of bit values programmed on each layer.

Barcoded lattices

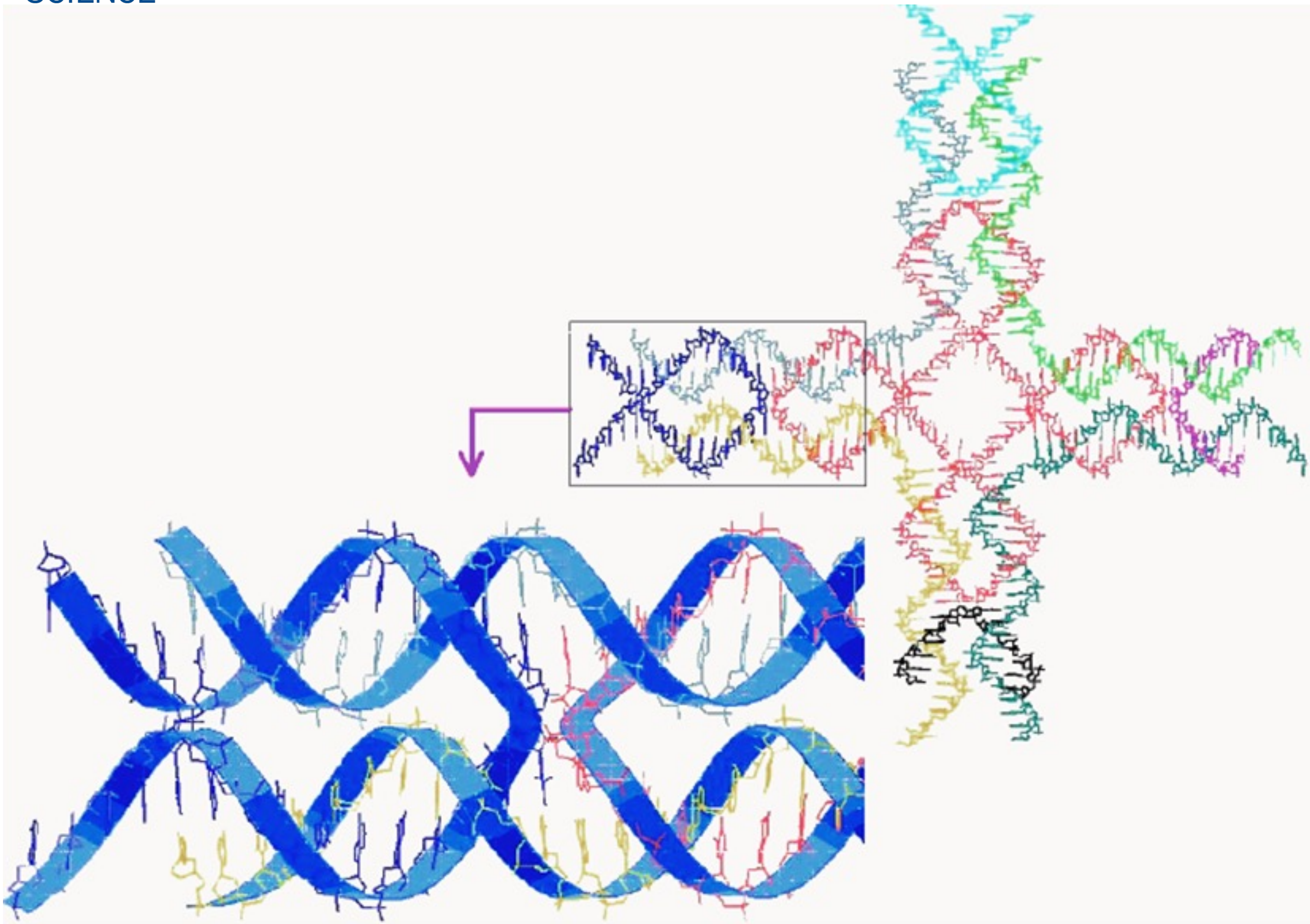


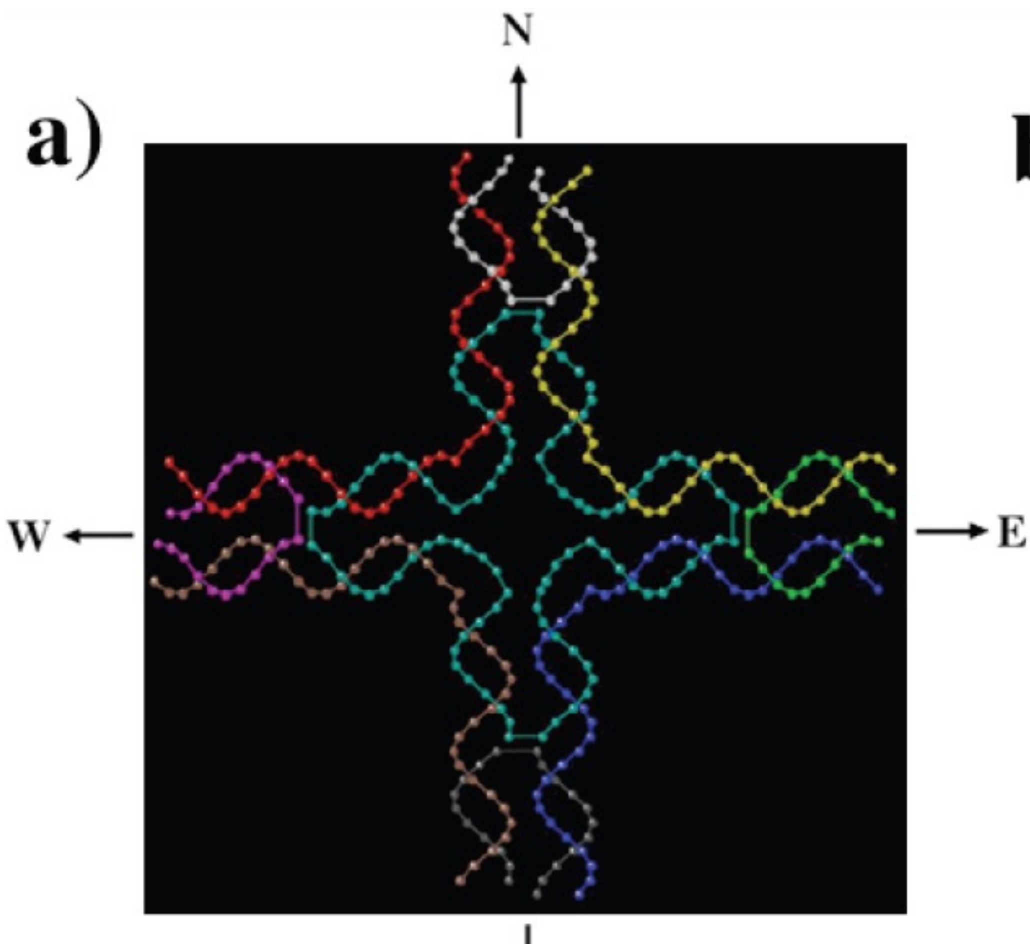
Cross Tiles and their DNA Lattices

DNA Cross Tile

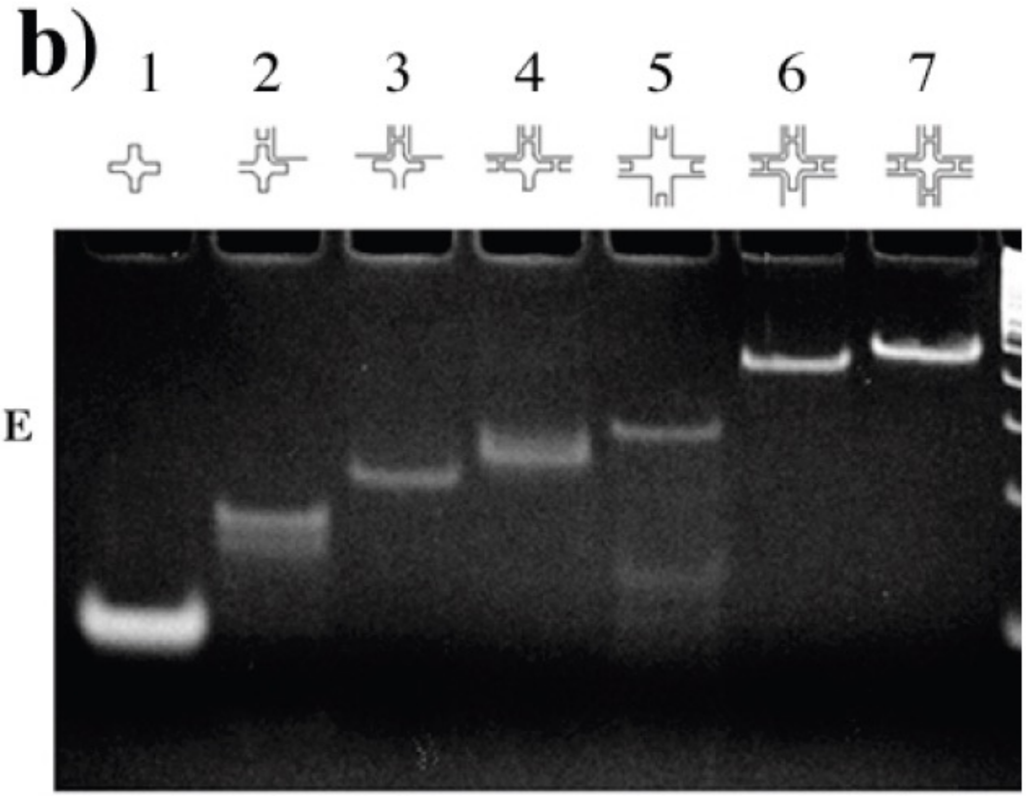


DNA Cross Tile





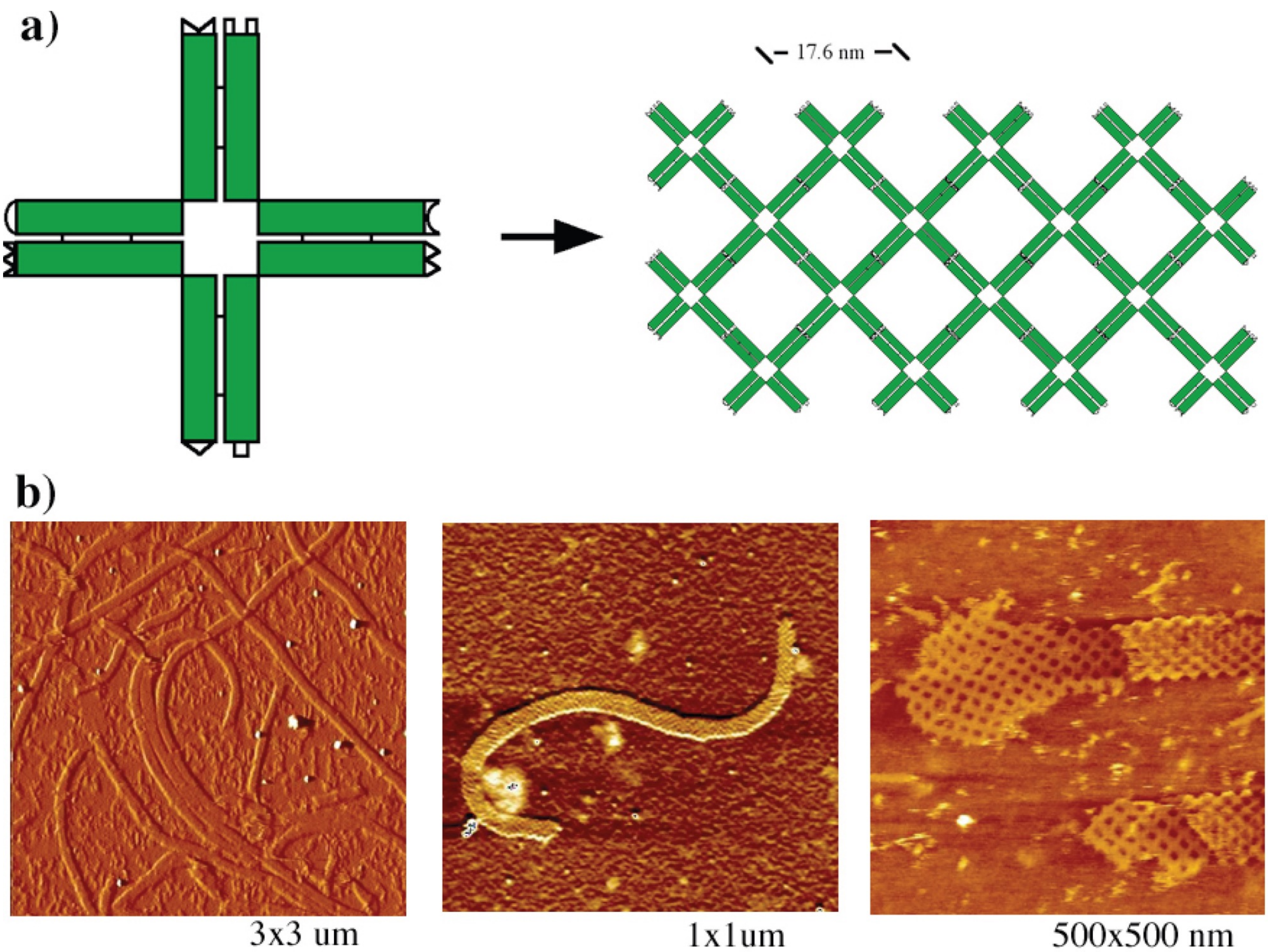
DNA Cross Tile



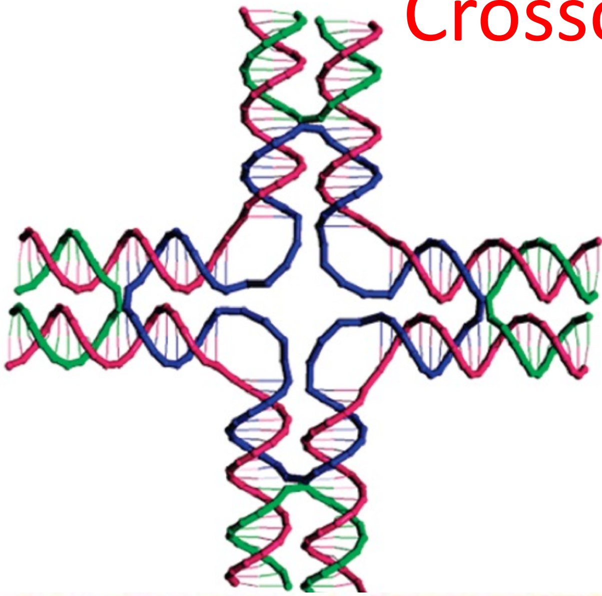
Gel Electrophoresis Data

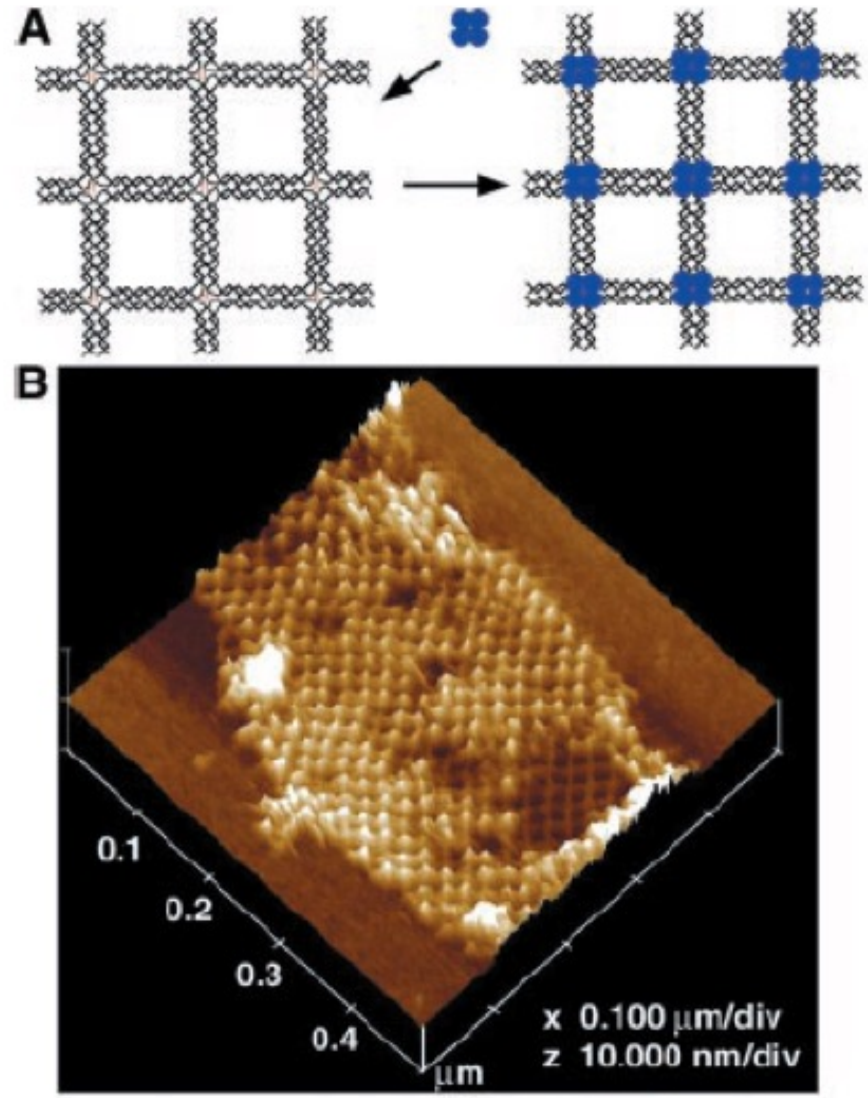
DUKE COMPUTER SCIENCE

Uncorrugated cross tile tubes

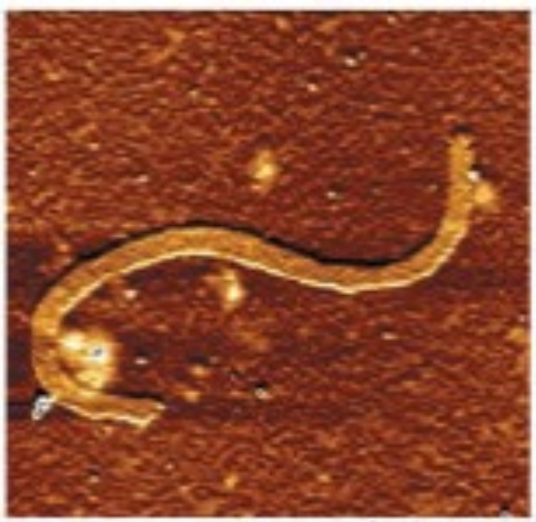


Crossover DNA Tiles and their Lattices



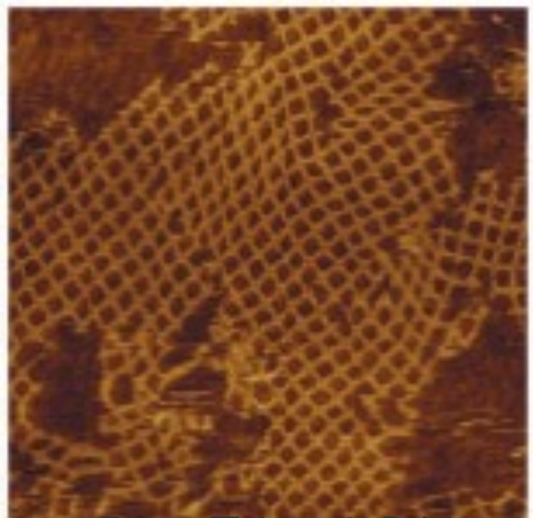


500x500nm



1x1 um

Naturally form Tube Lattices



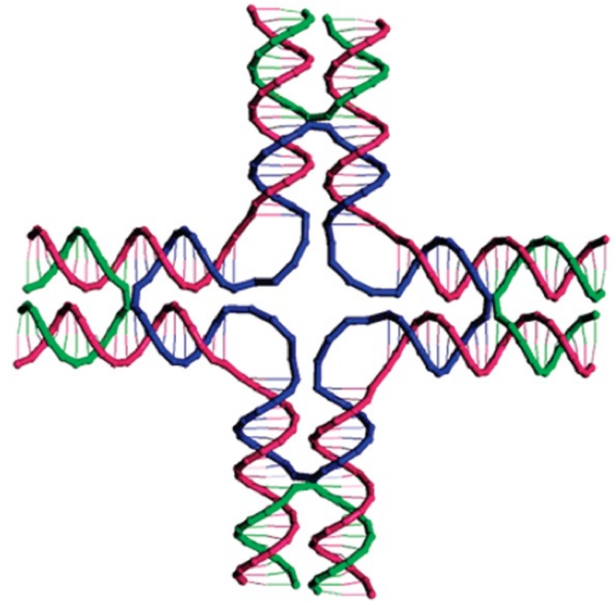
Form Tubes & Ribbons

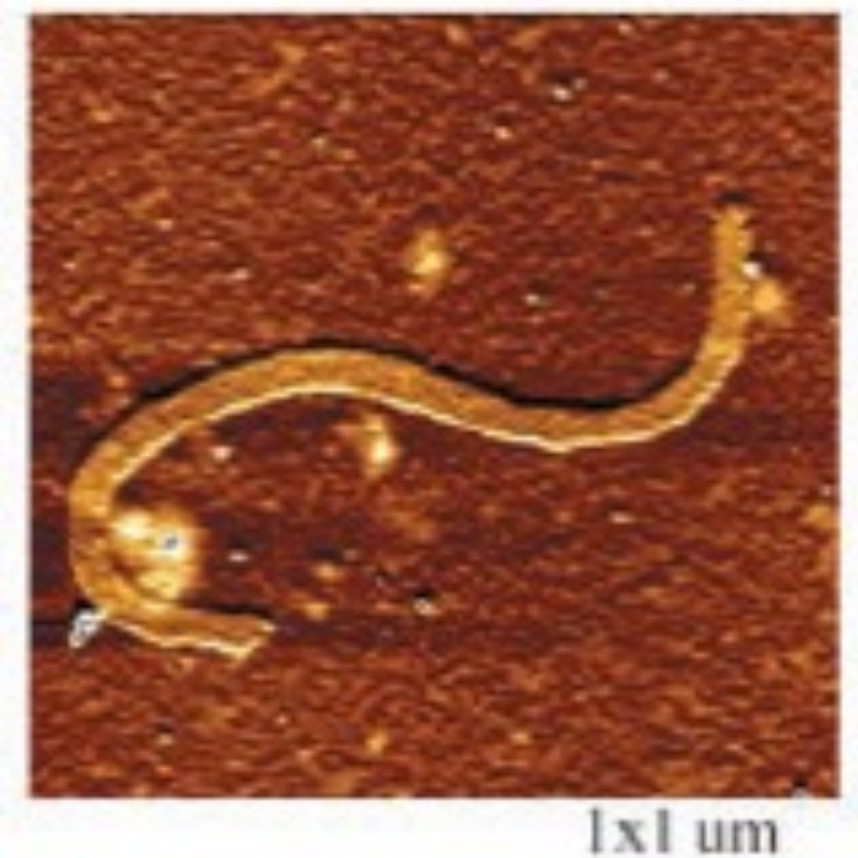
Used Corrugation to form 2D Grid Lattices

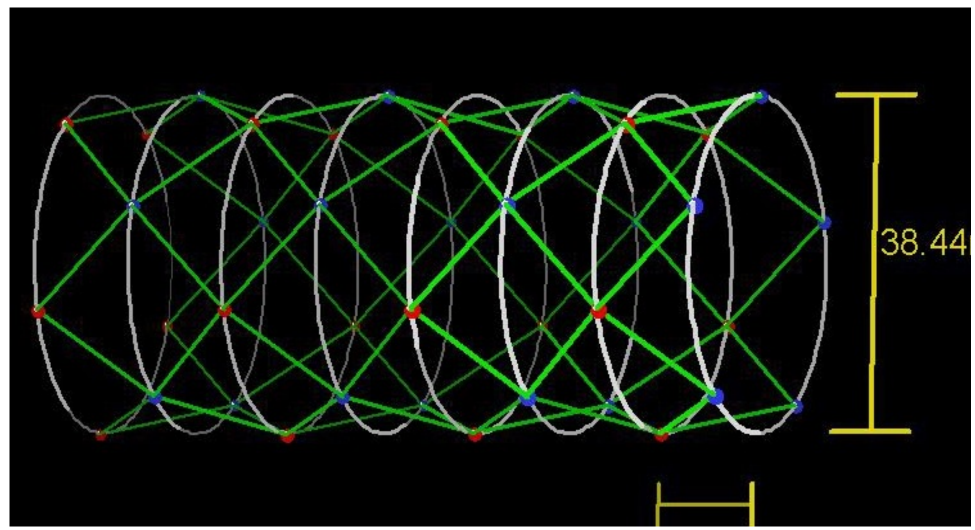
Hao Yan, Sung Ha Park, Liping Feng, John Reif, and Thomas H. LaBean, Science (2003)

Crossover DNA Tiles and their Lattices

Crossover DNA Tiles have some out-of-plate curvature, so naturally form Tube Lattices

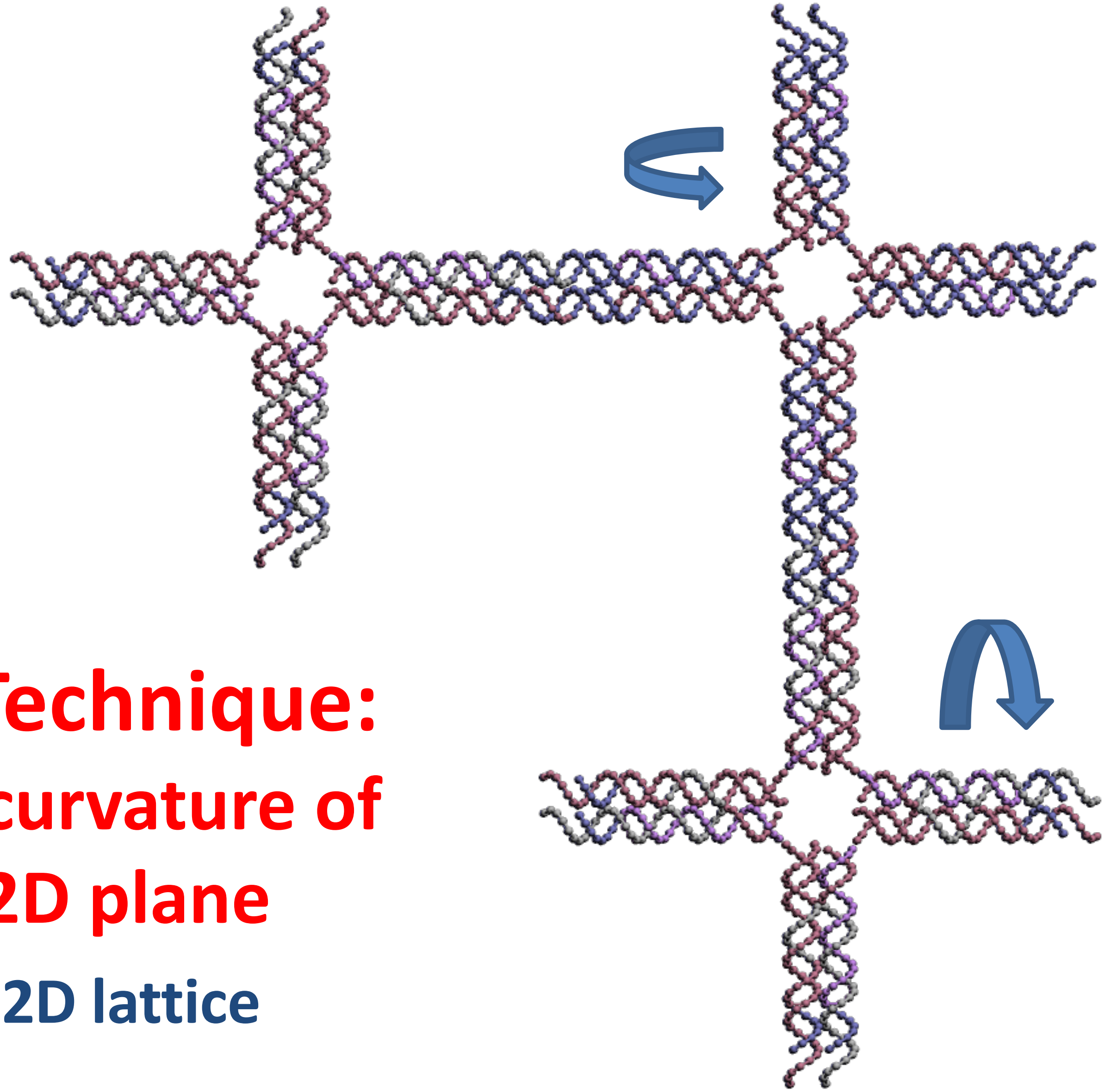






12.08nm

Tubes Self-Assembled from Uncorrugated Crossover tile:

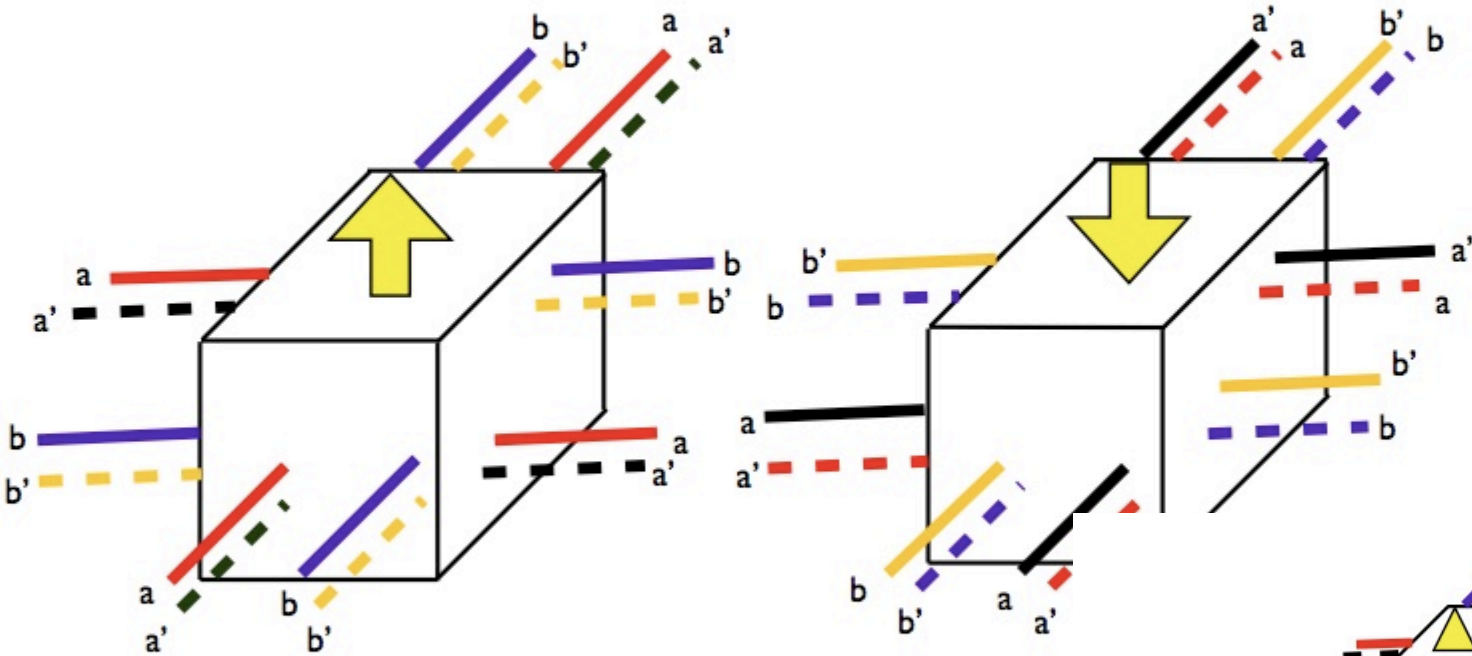


Corrugation Technique:

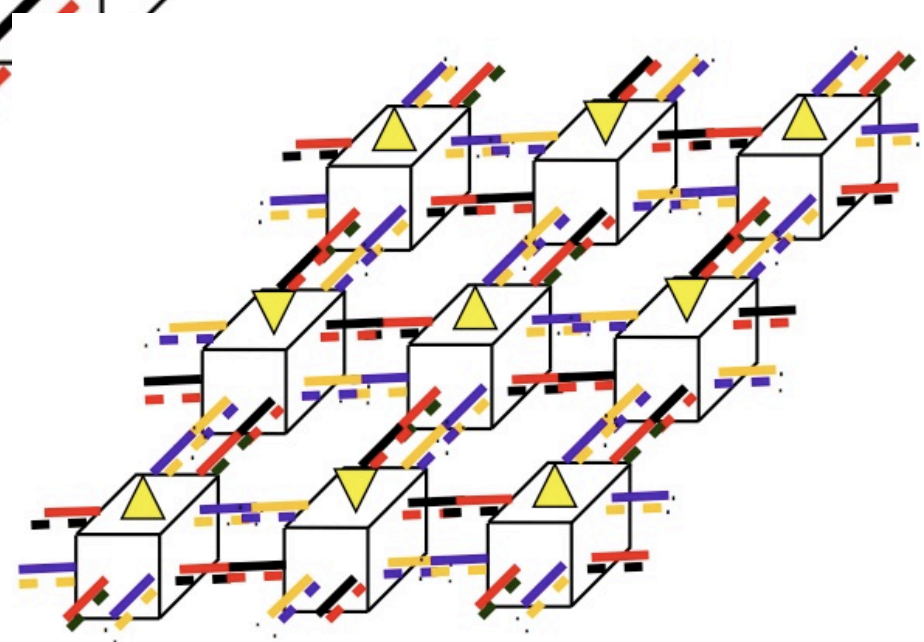
Used to cancel curvature of Tiles out of 2D plane

=> Results in a flat 2D lattice

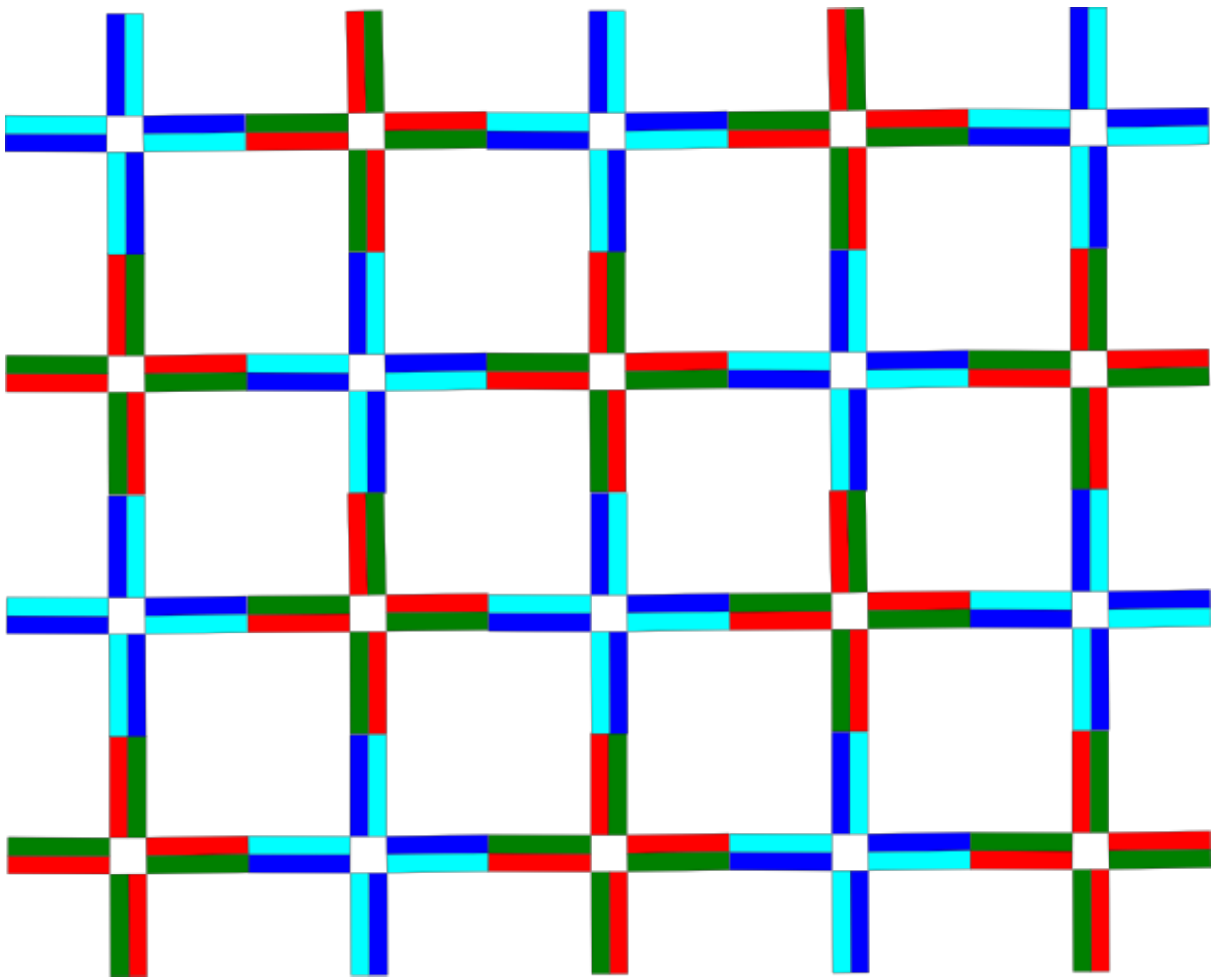
2D Corrugation to Cancel Lattice Curvature



2D Pad Programming of Crossover Tiles

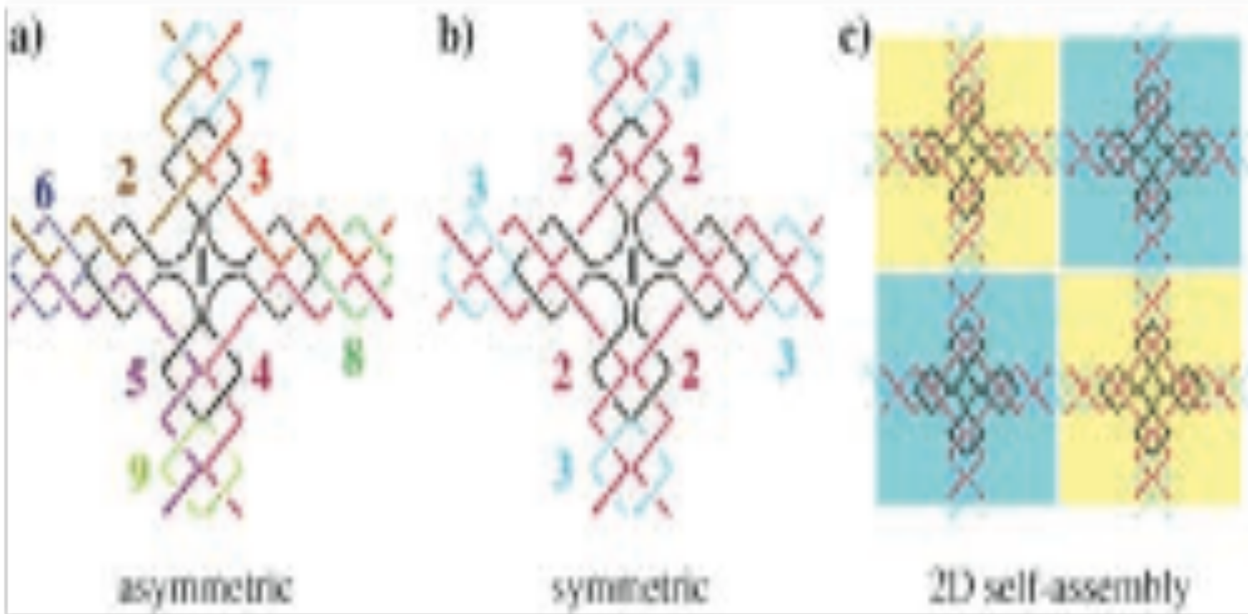


2D lattice design



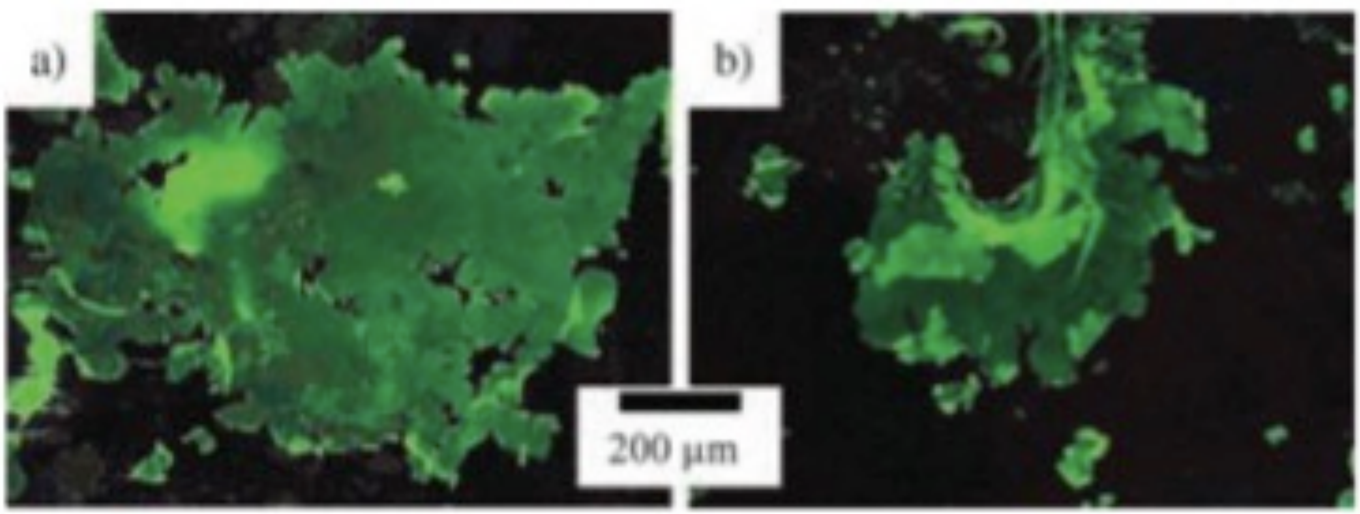
Corrugation

Cross tiles: Nano-Grid Assembly in 2D



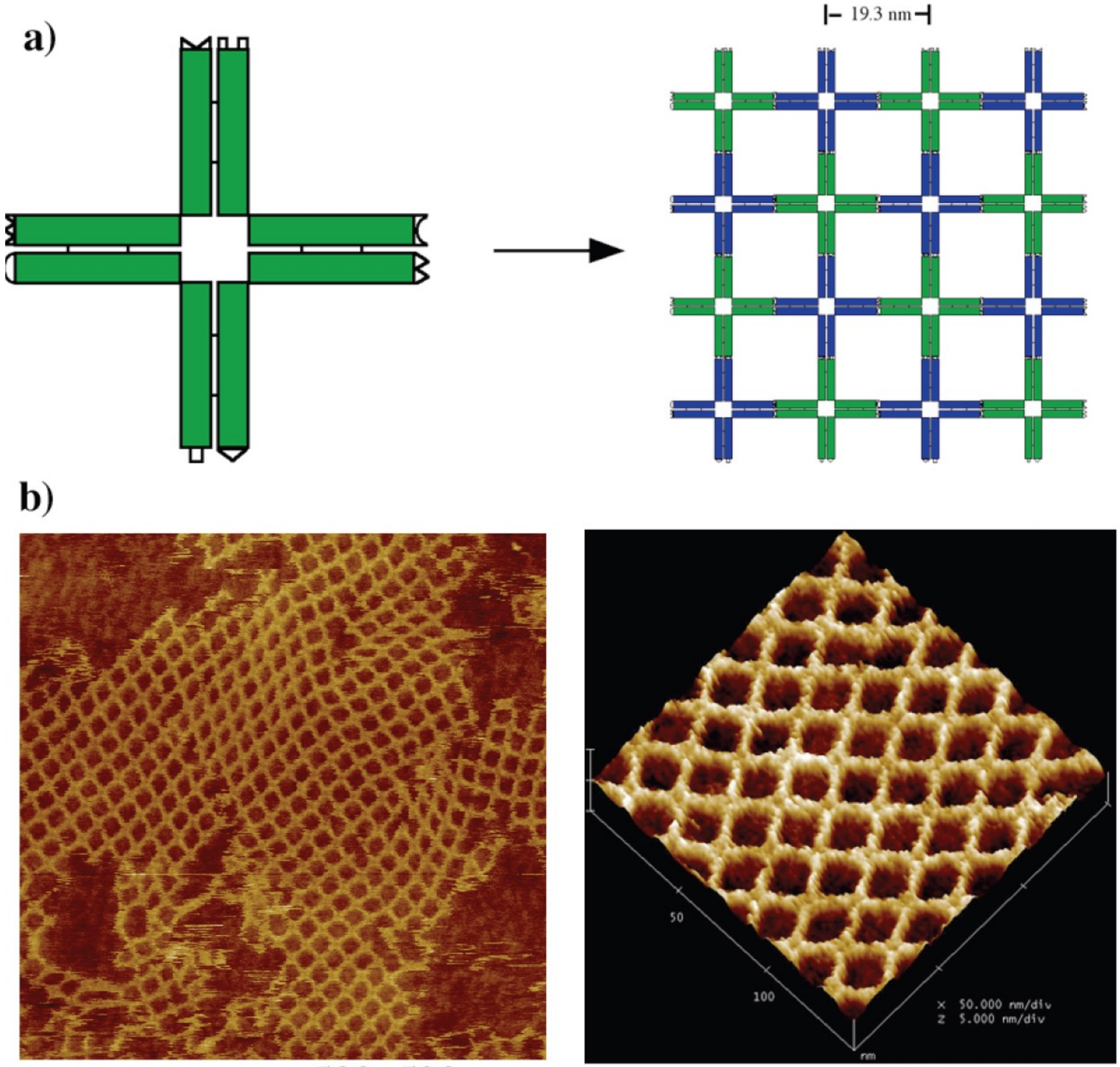
Figures adopted from He et al, 2005

Symmetric Cross Tiles



Corrugation allows creation of enormous lattices

Corrugated cross tile lattices

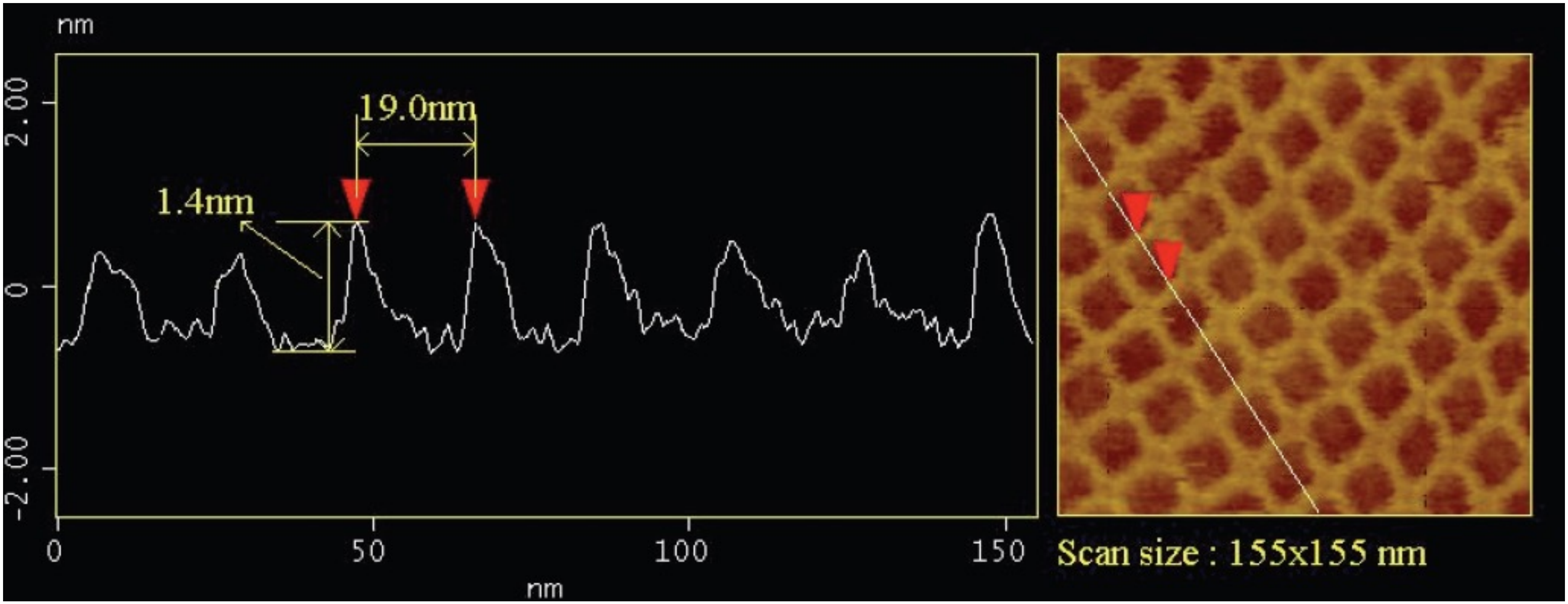


500x500nm 150x150nm

Hao Yan, Sung Ha Park, Gleb Finkelstein, John H. Reif, and Thomas H. LaBean, DNA-Templated Self-Assembly of Protein Arrays and Highly Conductive Nanowires, Science, Vol. 301, pp. 1882-1884, Sep 26 2003.

Corrugated cross tile lattices:

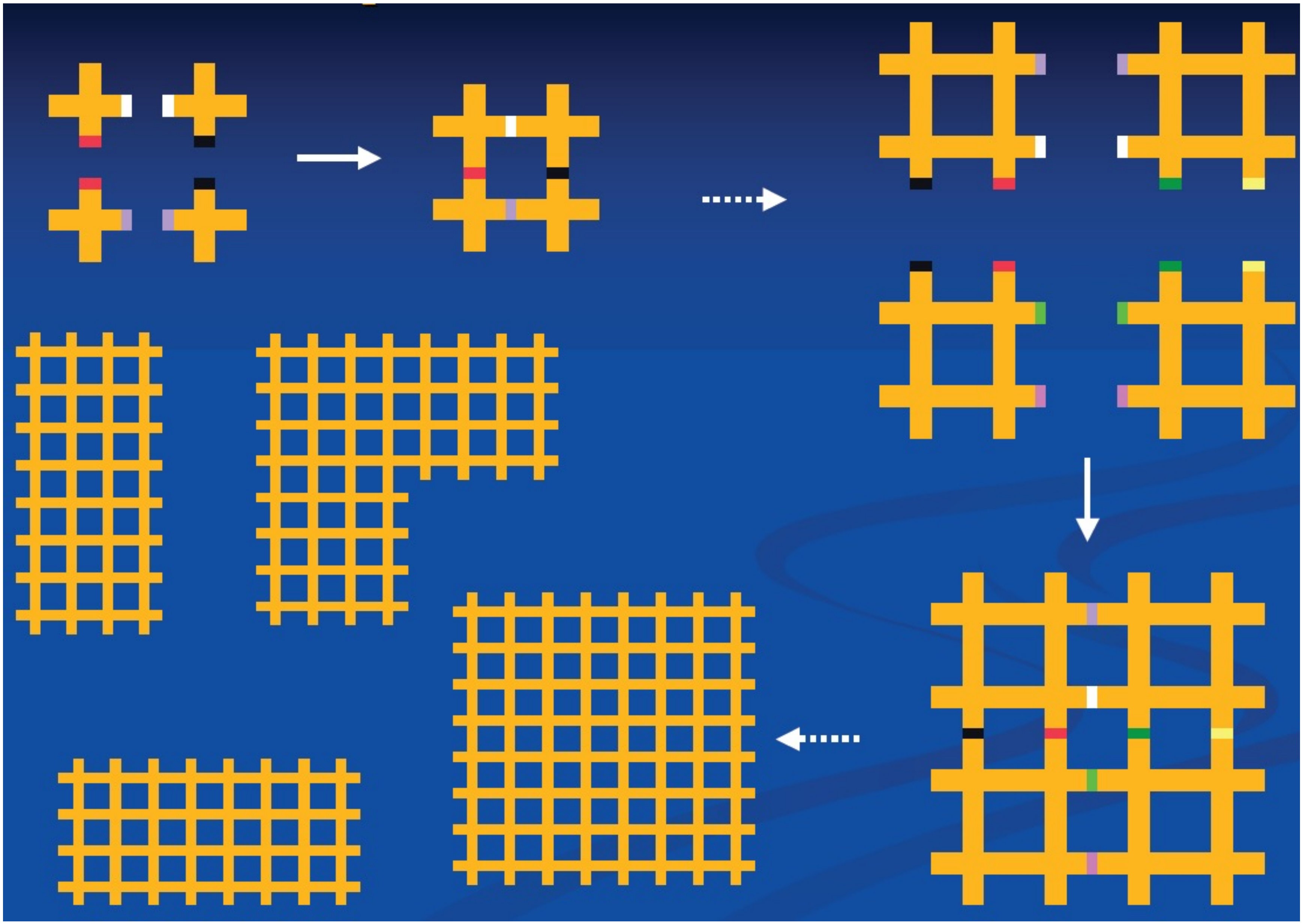
Highly uniform molecular scale lattices far below VLSI scales



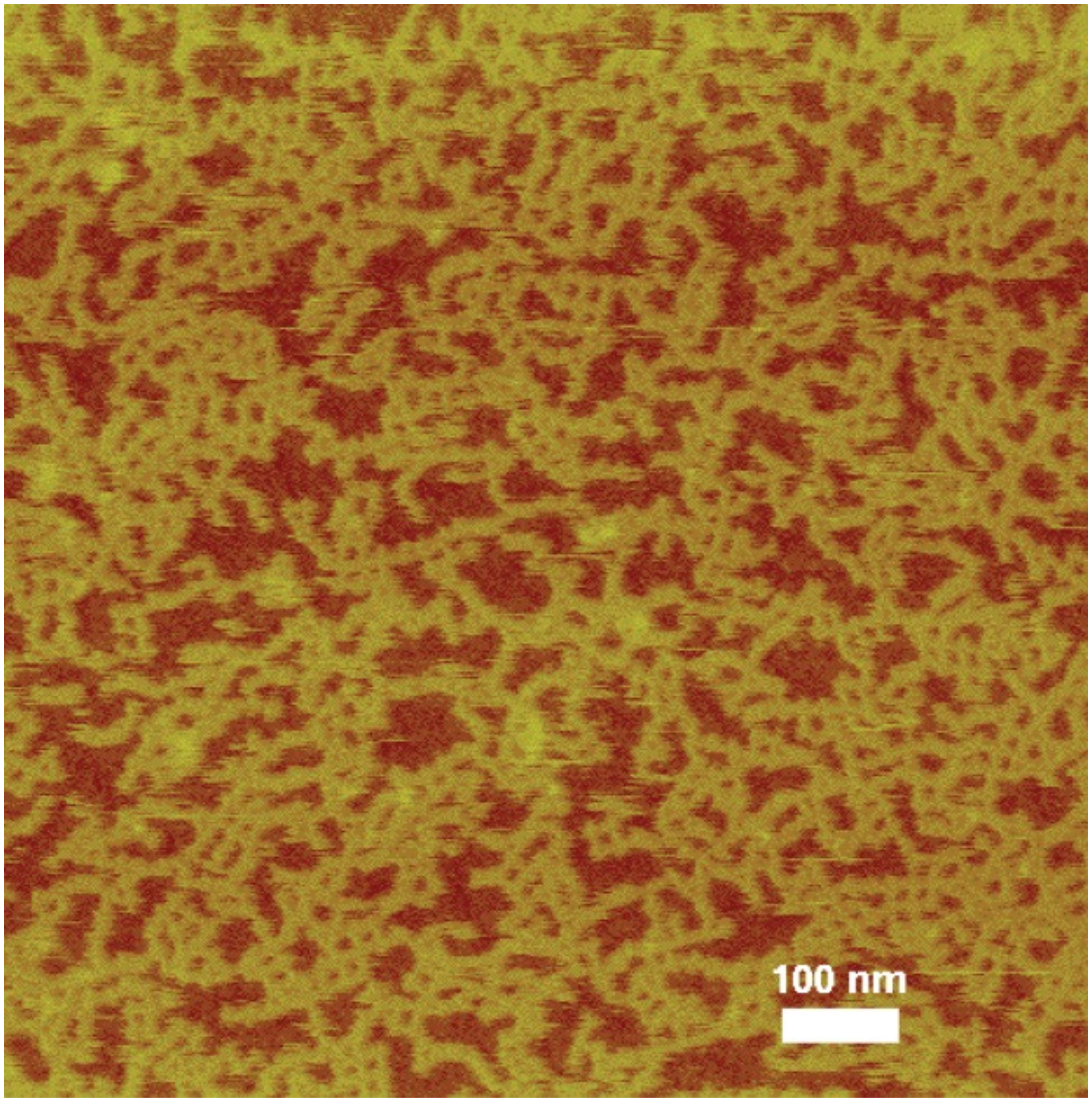
Hierarchical Tile Assemblies

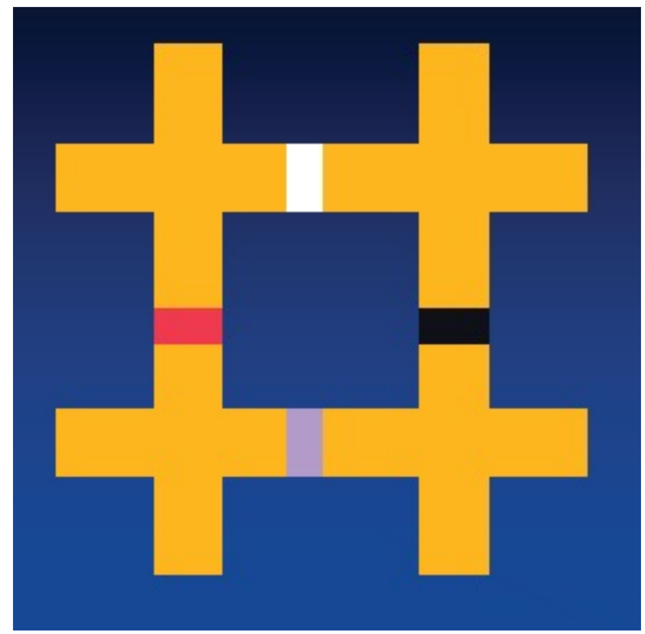
Sung Ha Park, Constantin Pistol, Sang Jung Ahn, John H. Reif, Alvin R. Lebeck, Chris Dwyer, and Thomas H. LaBean, Finite-Size, Fully Addressable DNA Tile Lattices Formed by Hierarchical Assembly Procedures, Angewandte Chemie [International Edition], 2006.

Hierarchical Lattices of cross tiles

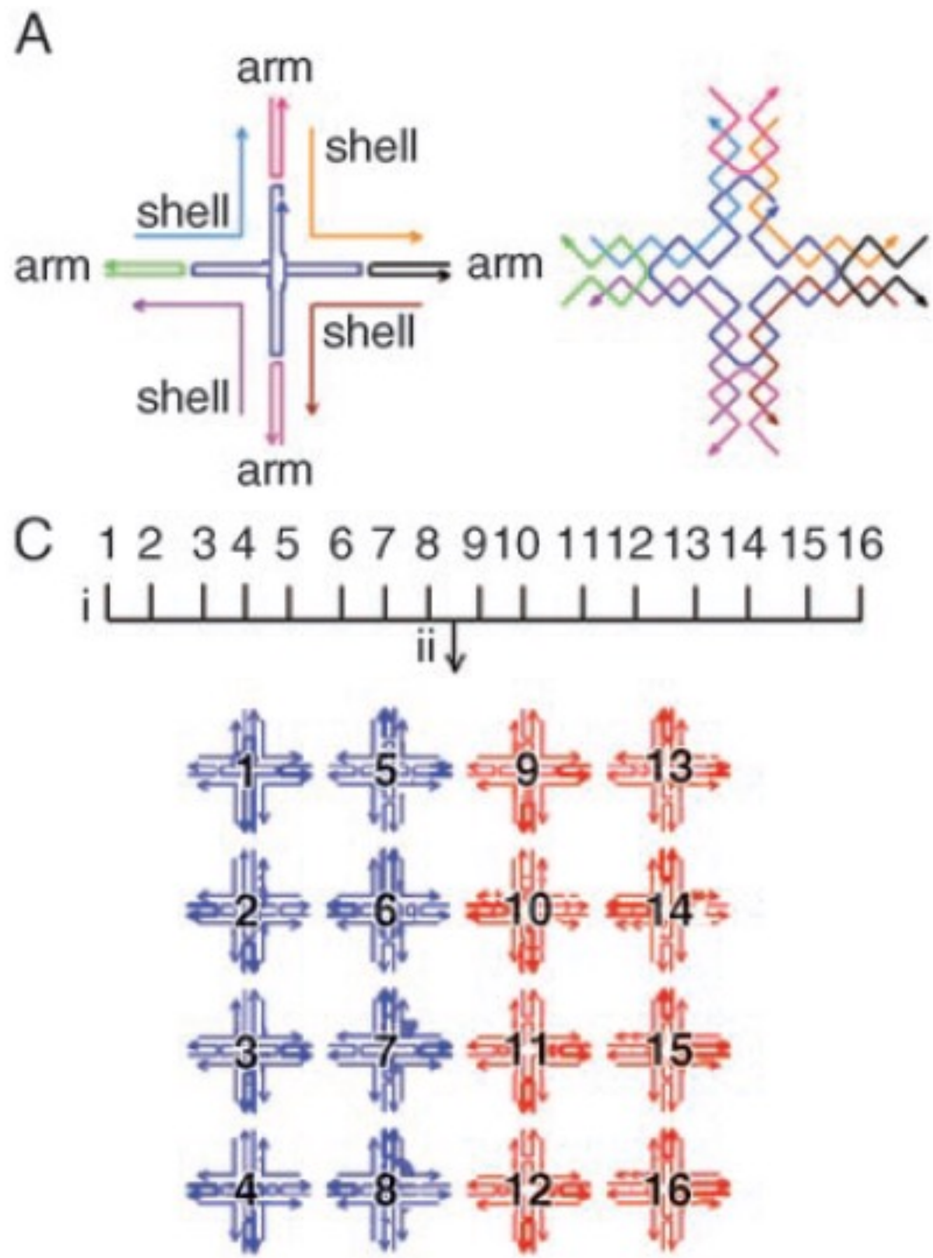


Hierarchical Assembly of cross tiles

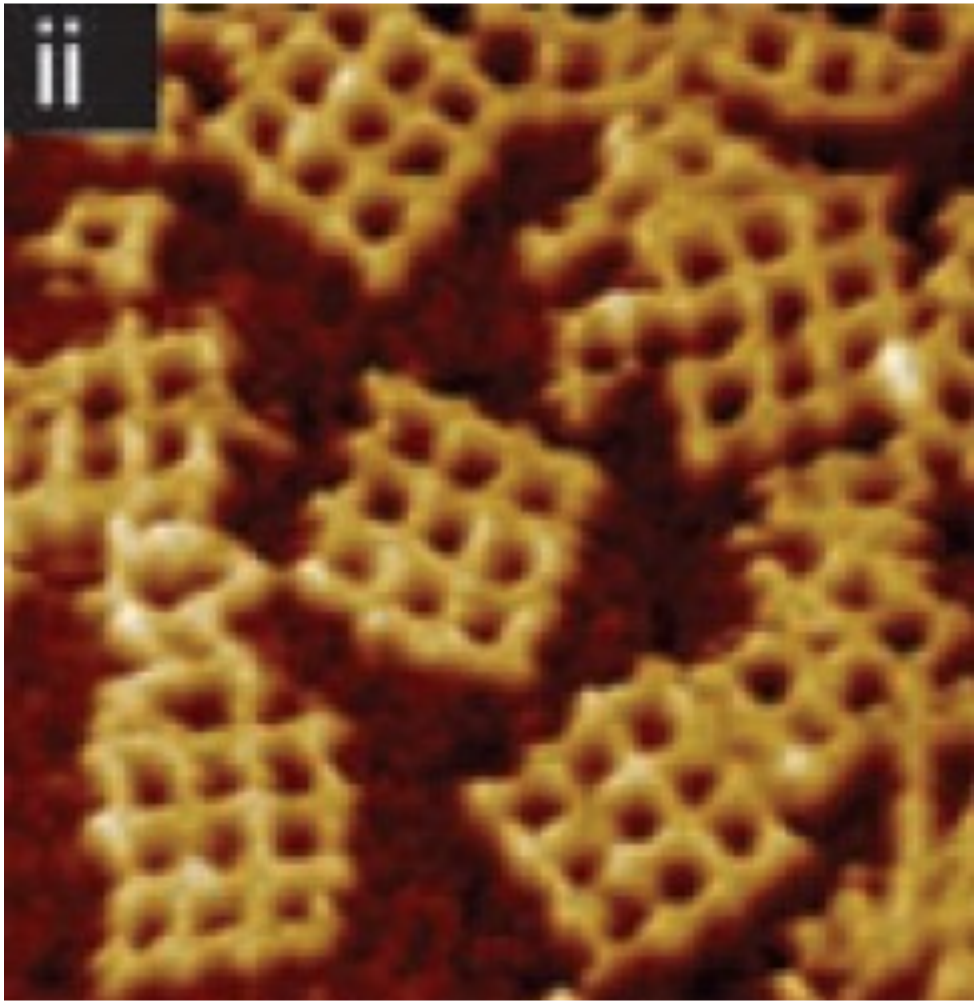


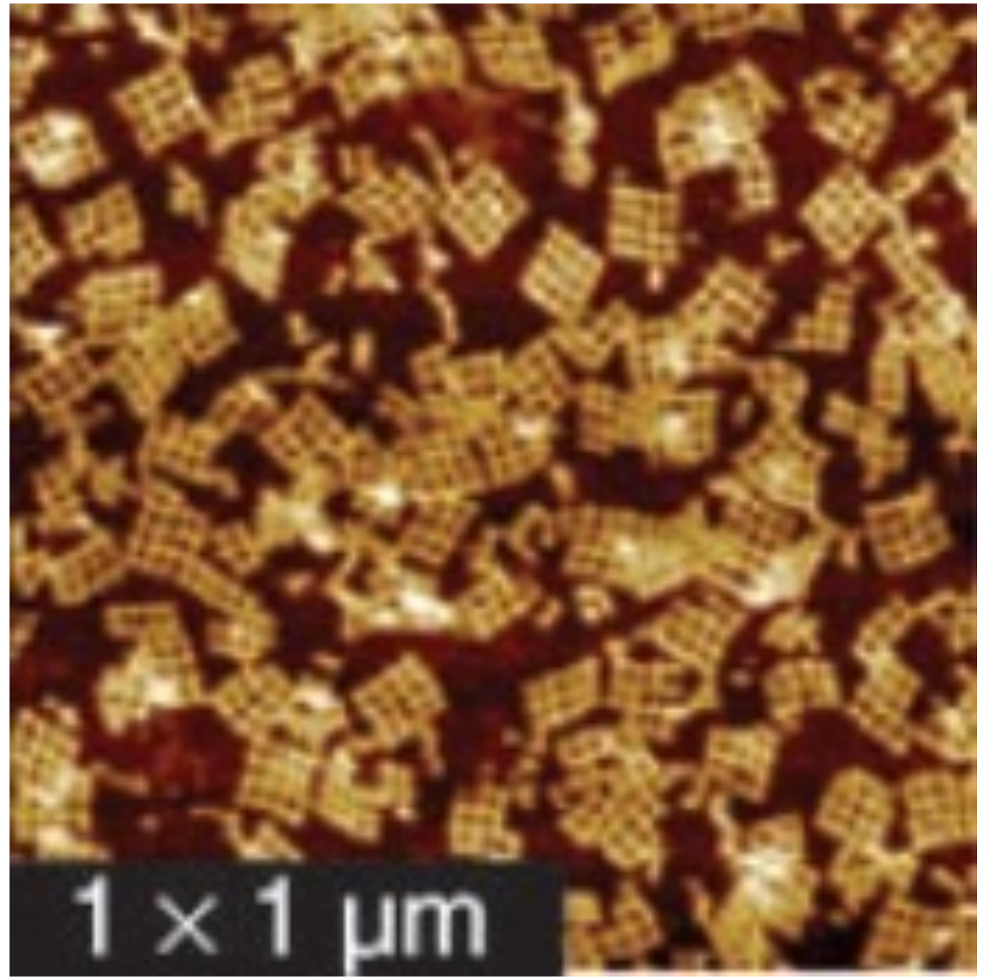


Addressable cross tiles used for Hierarchical Assembly



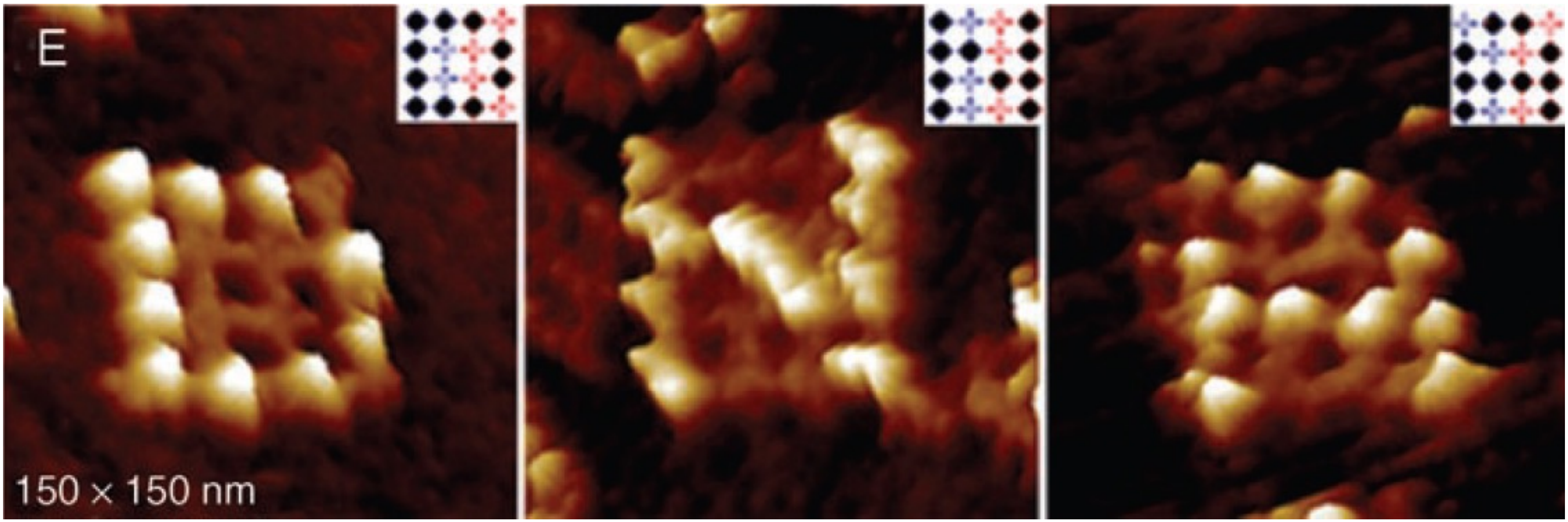
Addressable cross tiles used for Hierarchical Assembly



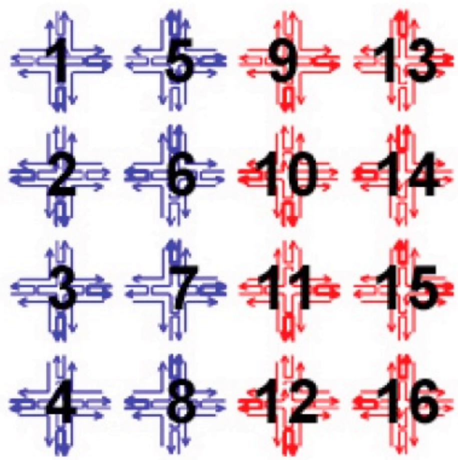


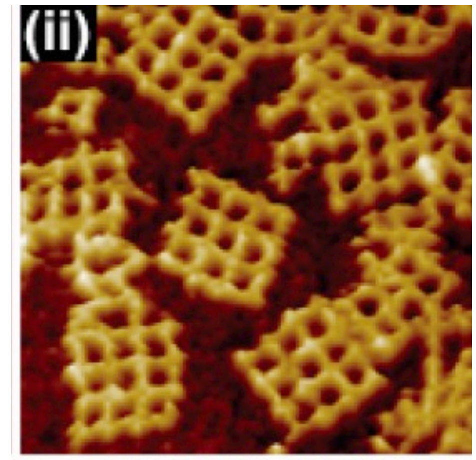
Sung Ha Park, Constantin Pistol, Sang Jung Ahn, John H. Reif, Alvin R. Lebeck, Chris Dwyer, and Thomas H. LaBean, Finite-Size, Fully Addressable DNA Tile Lattices Formed by Hierarchical Assembly Procedures, Angewandte Chemie [International Edition], Volume 45, Issue 5, pp. 735-739

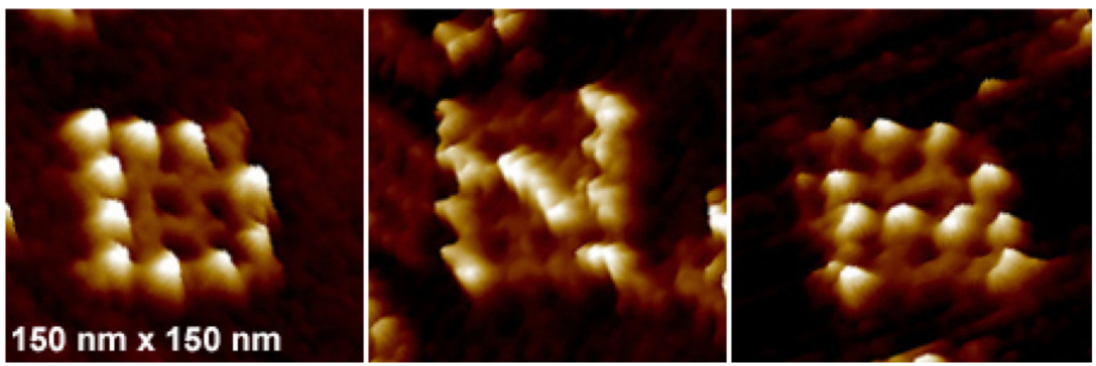
Molecular Scale Patterning using Hierarchical Assembly of cross tiles



Hierarchical Assembly of DNA Lattices with 2 D Pattern "DNA"

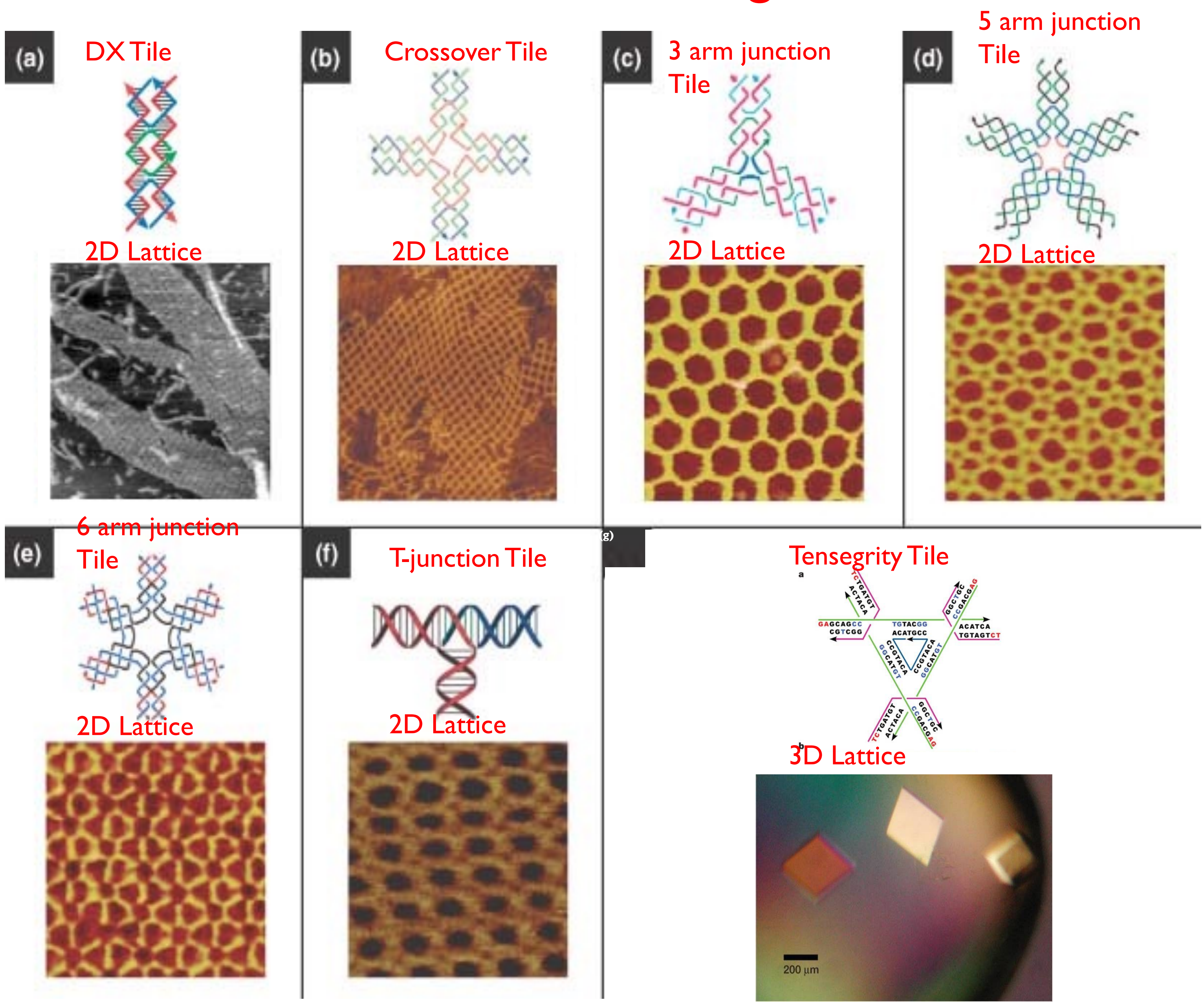






Sung Ha Park, Constantin Pistol, Sang Jung Ahn, John H. Reif, Alvin R. Lebeck, Chris Dwyer, and Thomas H. LaBean, Finite-Size, Fully Addressable DNA Tile Lattices Formed by Hierarchical Assembly Procedures, Angewandte Chemie [International Edition], 2006.

Diverse DNA Tiles and Resulting DNA Lattices



Double Decker Tiles and 3D DNA Lattices

Urmi Majumder, Duke

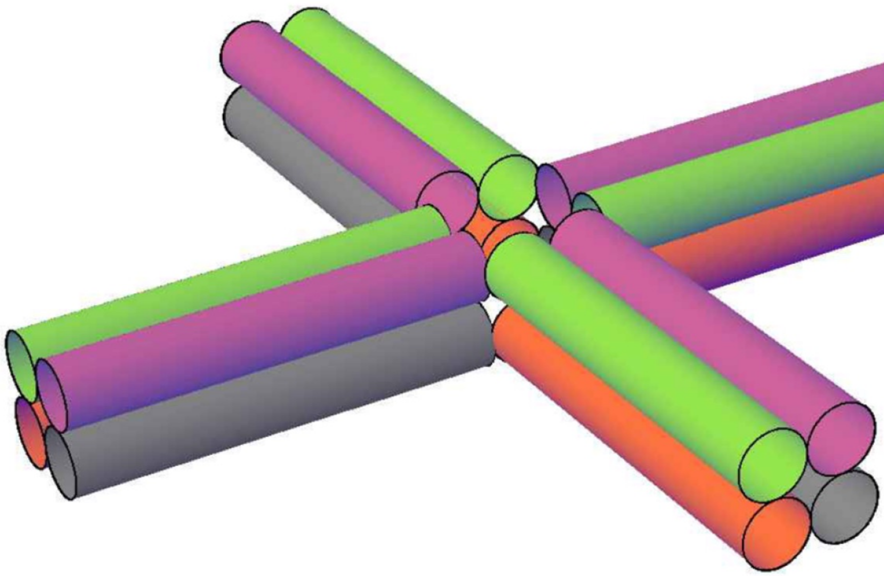
Urmi Majumdar, Abhijit Rangnekar, Kurt V. Gothelf, John H Reif and Thomas H LaBean, Design and Construction of Double-Decker Tile as a Route to Three-Dimensional Periodic Assembly of DNA, Journal American Chemical Society (JACS), Vol. 133, no. 11, pp. 3843—3845 (Feb. 2011)

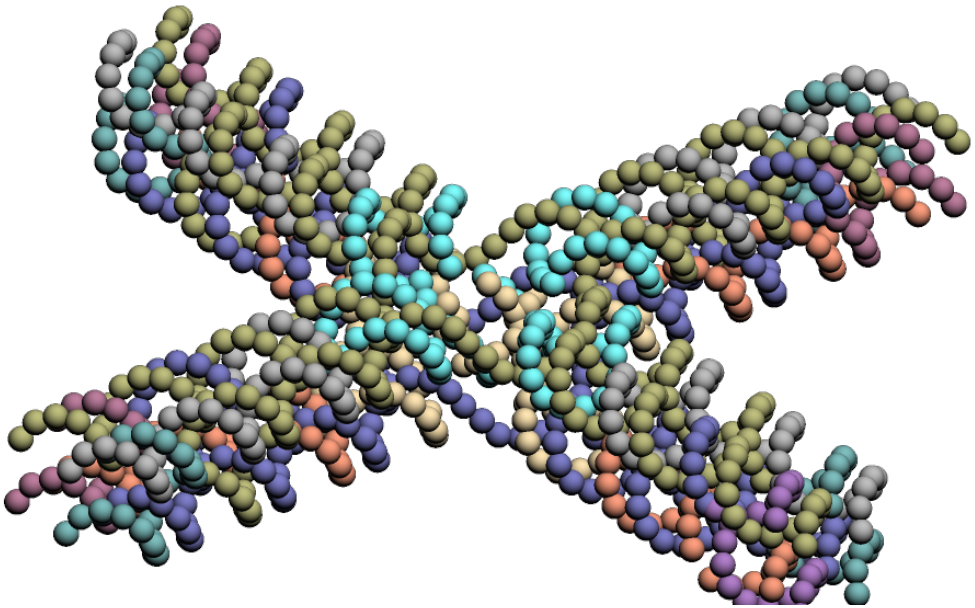
Application of 3D lattices:

- Imaging proteins
- Organizing molecular electronic components
- Organizing functional inorganic materials
- Tile based computing

Double decker tiles:

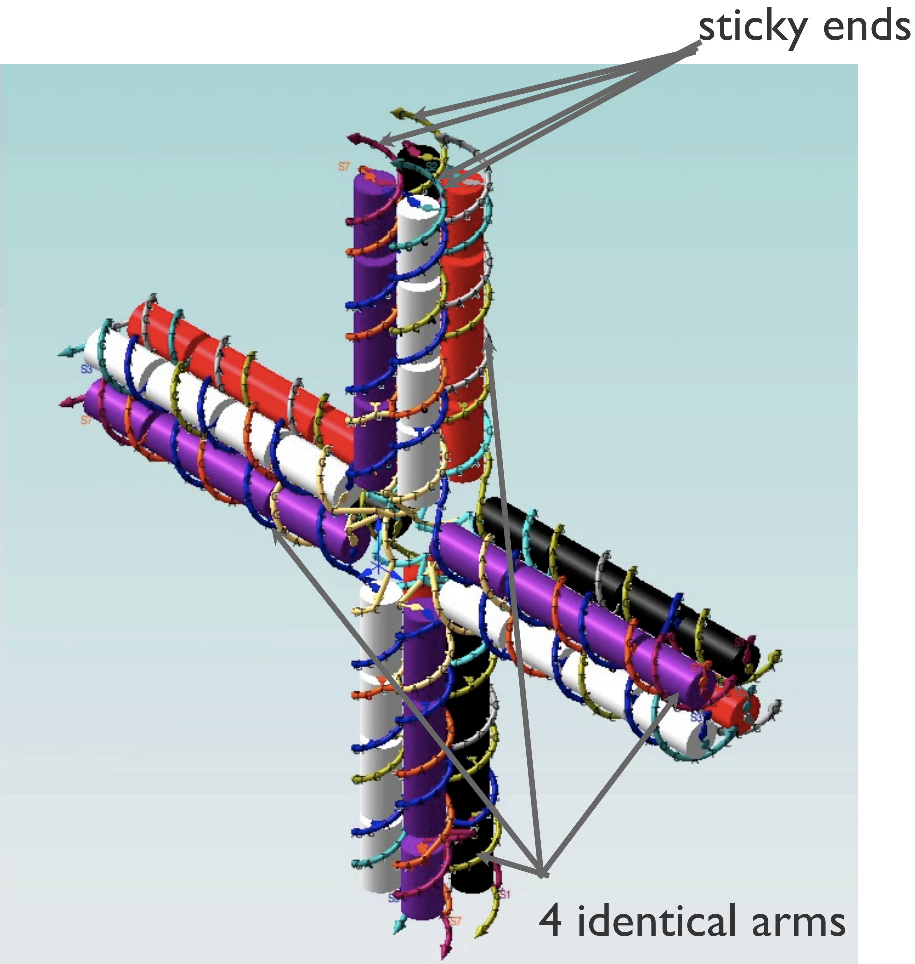
Used for 3D DNA Lattices

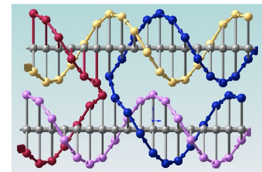




Four fold sequence symmetry

Double-decker tiles: Route to Assembly in 3D





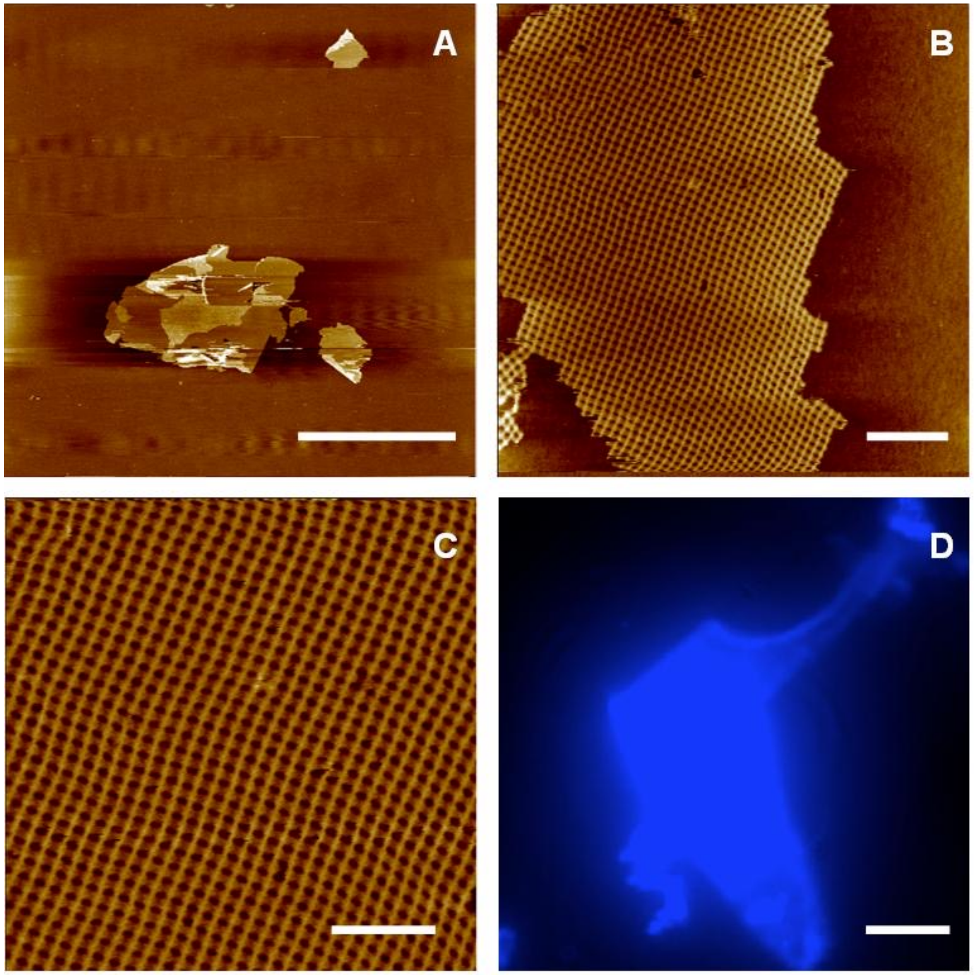
Branched Junction

2 cross tiles held together by branched junctions

Urmi Majumder, Duke

DUKE COMPUTER SCIENCE

Highly regular 2D lattices via double decker cross tiles



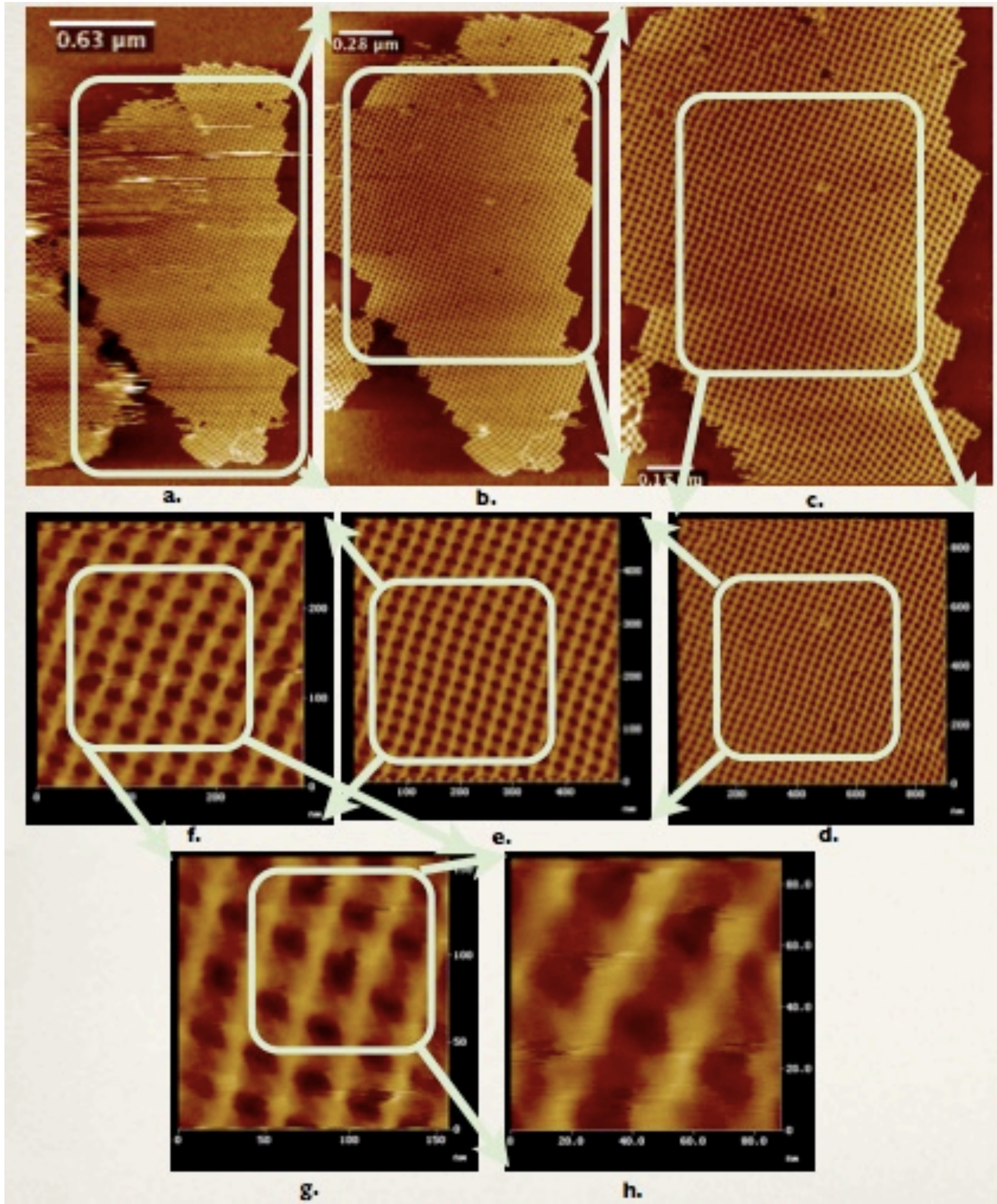
Atomic force microscopy images of the double-decker 2D lattice with corrugation.
The lattices are tens of micrometers in size.

The scale bars are:
(A) 10 µm,
(B) 300 nm
(C) 200 nm.
(D) Fluorescence microscopy image of the same sample. (The scale bar is 20 µm).

Urmi Majumder, Abhijit Rangnekar, Kurt V. Gothelf, John H. Reif and Thomas H. LaBean, Design and Construction of Double-Decker Tile as a Route to Three-Dimensional Periodic Assembly of DNA. J. Am. Chem. Soc., 2011, 133 (11), pp 3843–3845

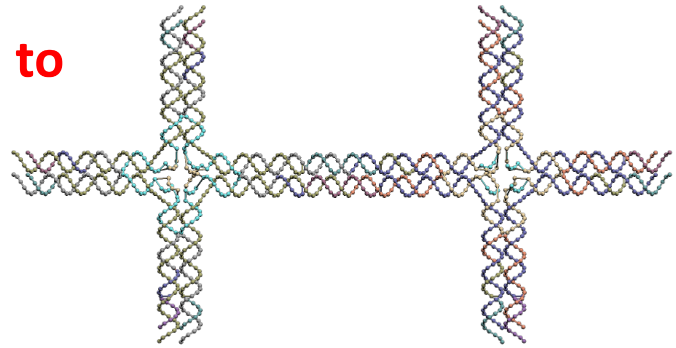
2D Lattices using Double-decker tiles

Extremely Large, Regular 2D Grids
with Predominant Unidirectional Banding

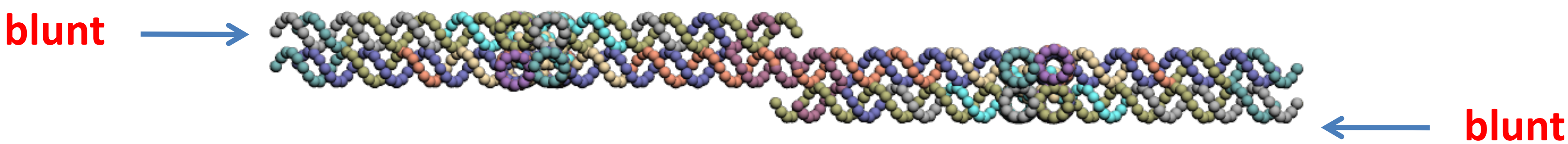


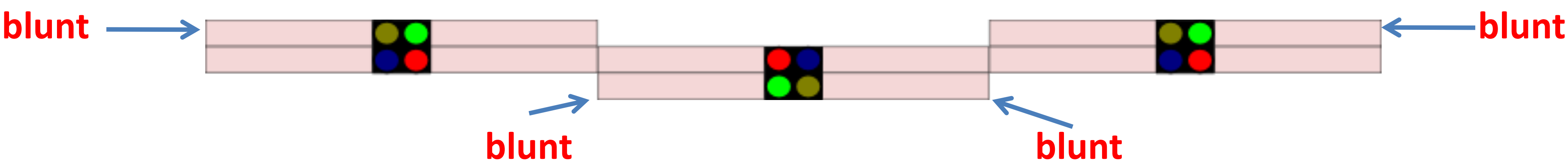
2D Staggered Lattices using Double-decker tiles

Use Corrugation to make flat in 2D:

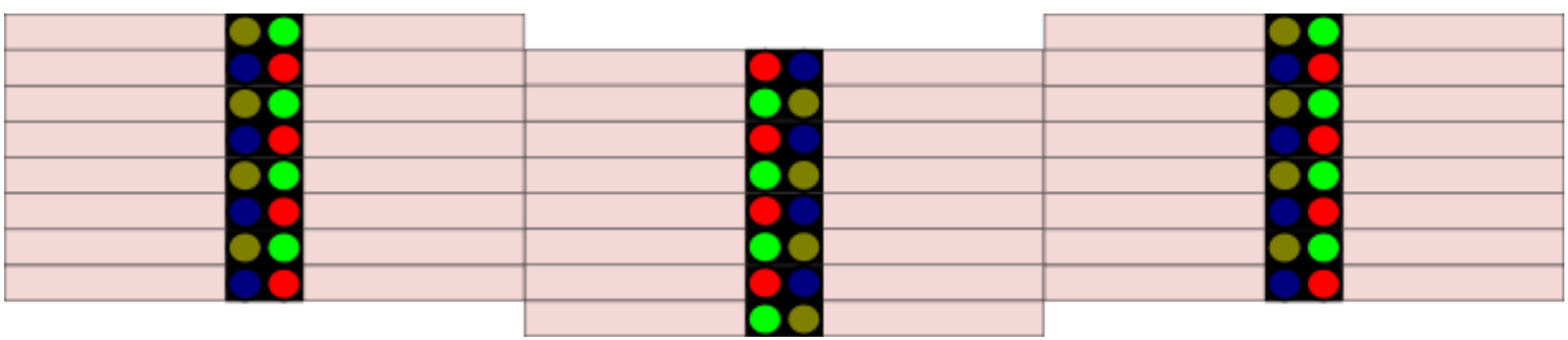


Staggered Attachments:





3D Lattice using Staggered Attachments:



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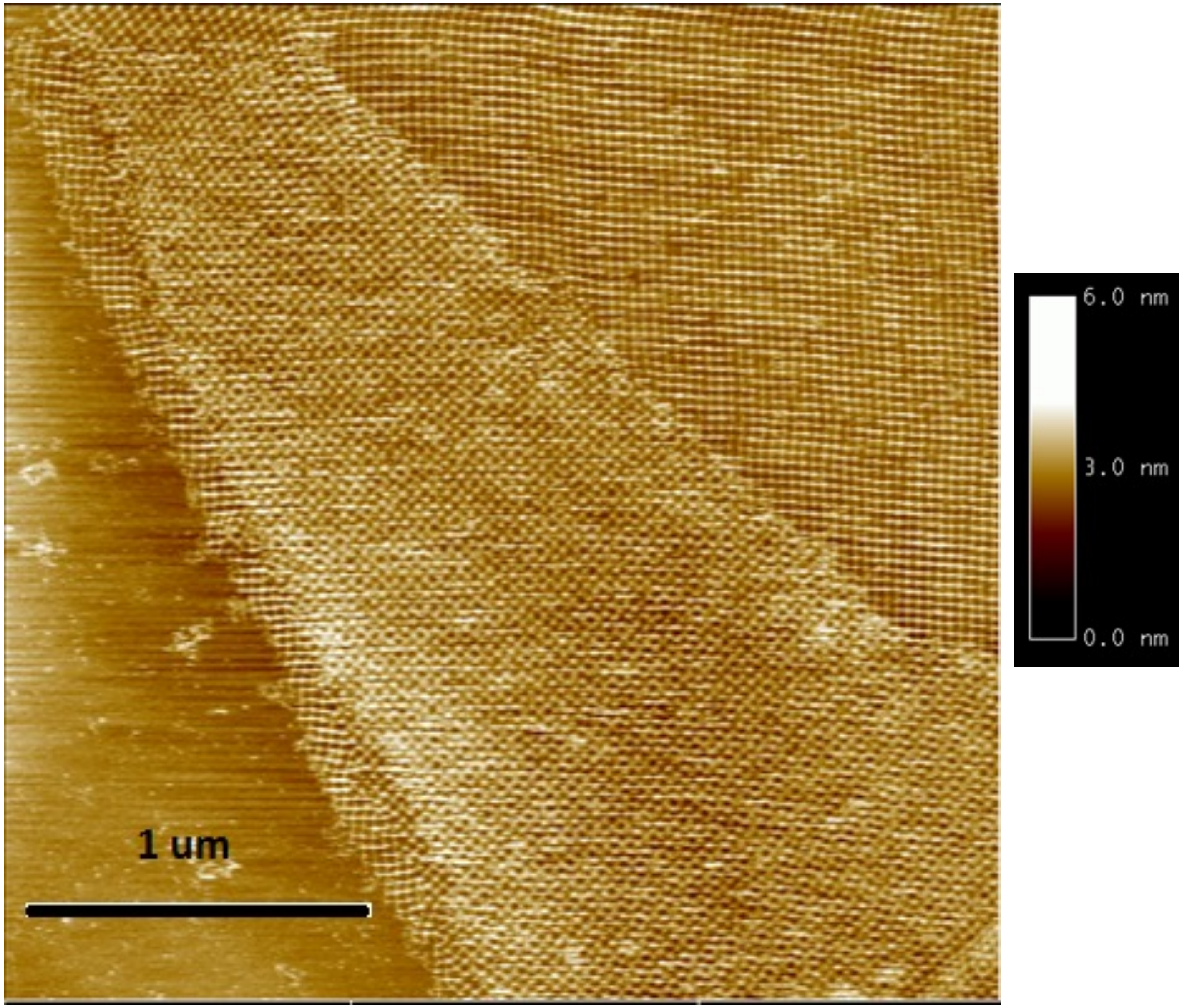
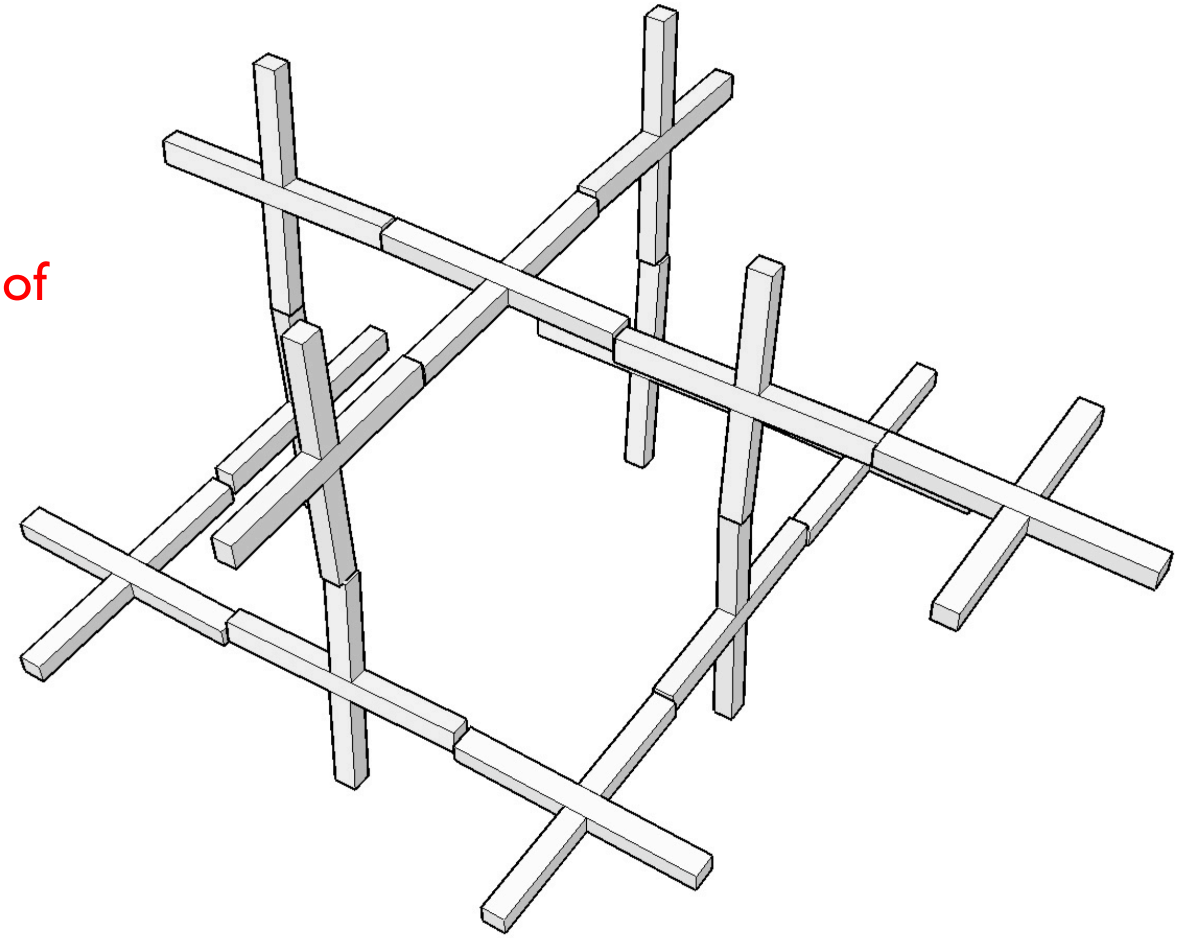
2D staggered lattices AFM



Double-decker tiles: forming 3D Lattices

3D Arrangement of Double-Decker Tiles



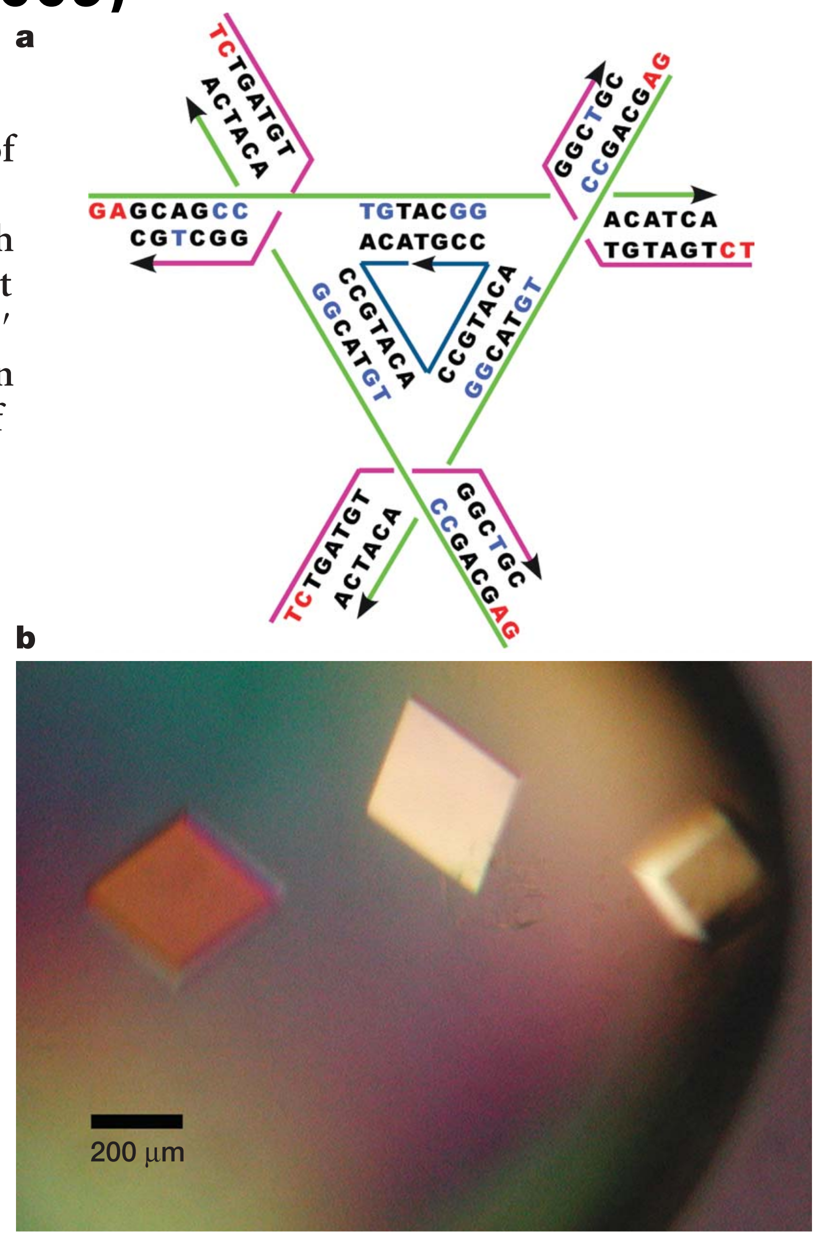
3D Generalized Corrugation cancels curvature of lattice in all 3 dimensions !

Urmi Majumder, Duke

Tensegrity Tiles & 3D lattices

(Seeman, Nature, 2009)

Figure 1 | Schematic design, sequence, and crystal pictures. a, Schematic of the tensegrity triangle. The three unique strands are shown in magenta (strands restricted to a single junction), green (strands that extend over each edge of the tensegrity triangle) and dark blue (one unique nicked strand at the centre passing through all three junctions). Arrowheads indicate the 3′ ends of strands. Nucleotides with A-DNA-like characteristics are written in bright blue. Cohesive ends are shown in red letters. **b**, An optical image of crystals of the tensegrity triangle. The rhombohedral shape of the crystals and the scale are visible.



Seeman's Tensegrity tiles & 3D lattices

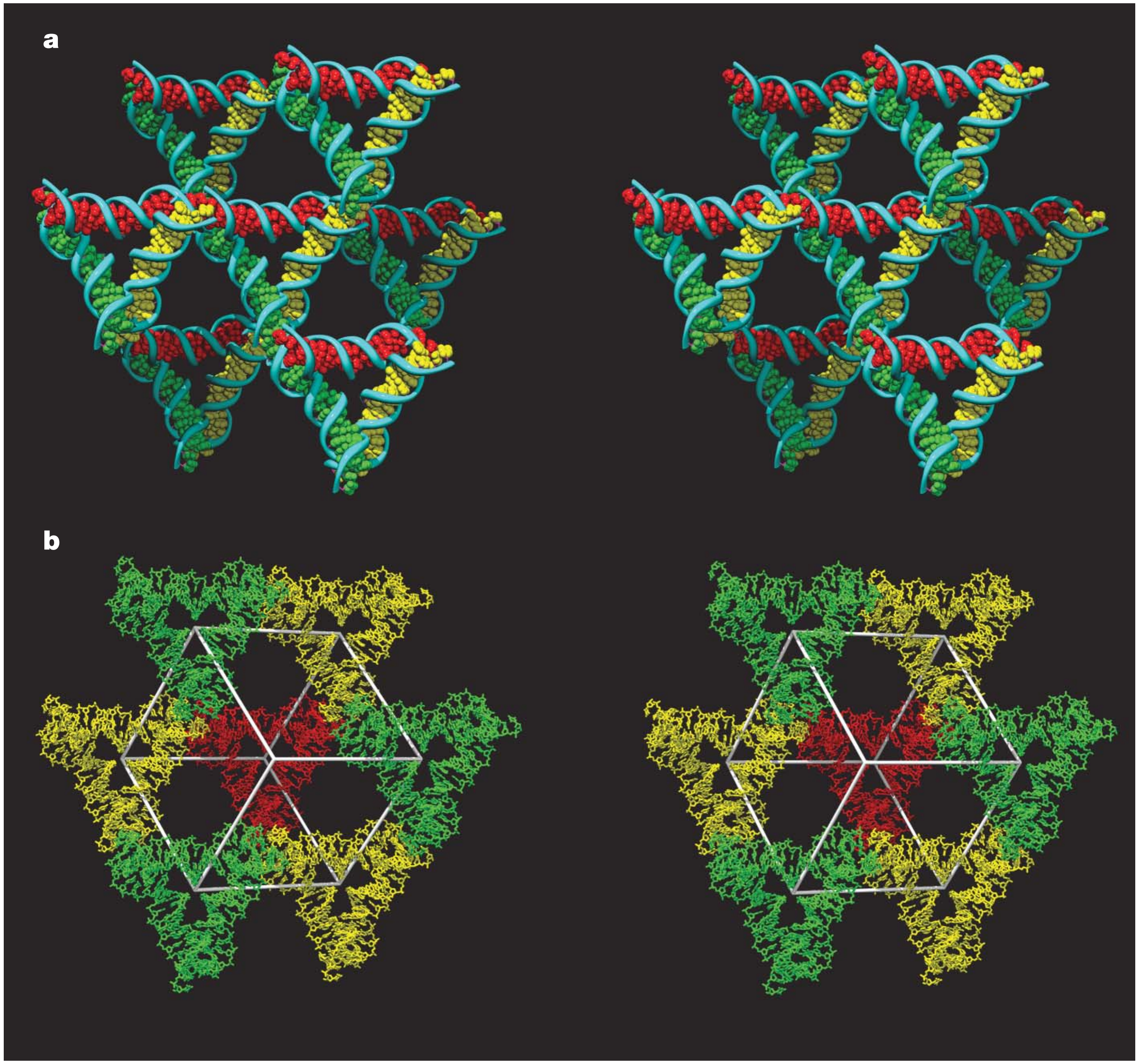


Figure 3 | Lattice formed by tensegrity triangles. a, Surroundings of a triangle. This stereoscopic image distinguishes three independent directions by base-pair colour. The central triangle is flanked by six other triangles. **b**, Rhombohedral cavity formed by tensegrity triangles. This stereoscopic image shows seven of the eight triangles that comprise the rhombohedron's corners. The cavity outline is drawn in white. The rear red triangle connects through one edge each to the three yellow triangles in a plane closer to the viewer. The yellow triangles are connected through two edges each to two different green triangles that are even nearer to the viewer.

Seeman's Tensegrity tiles & 3D lattices

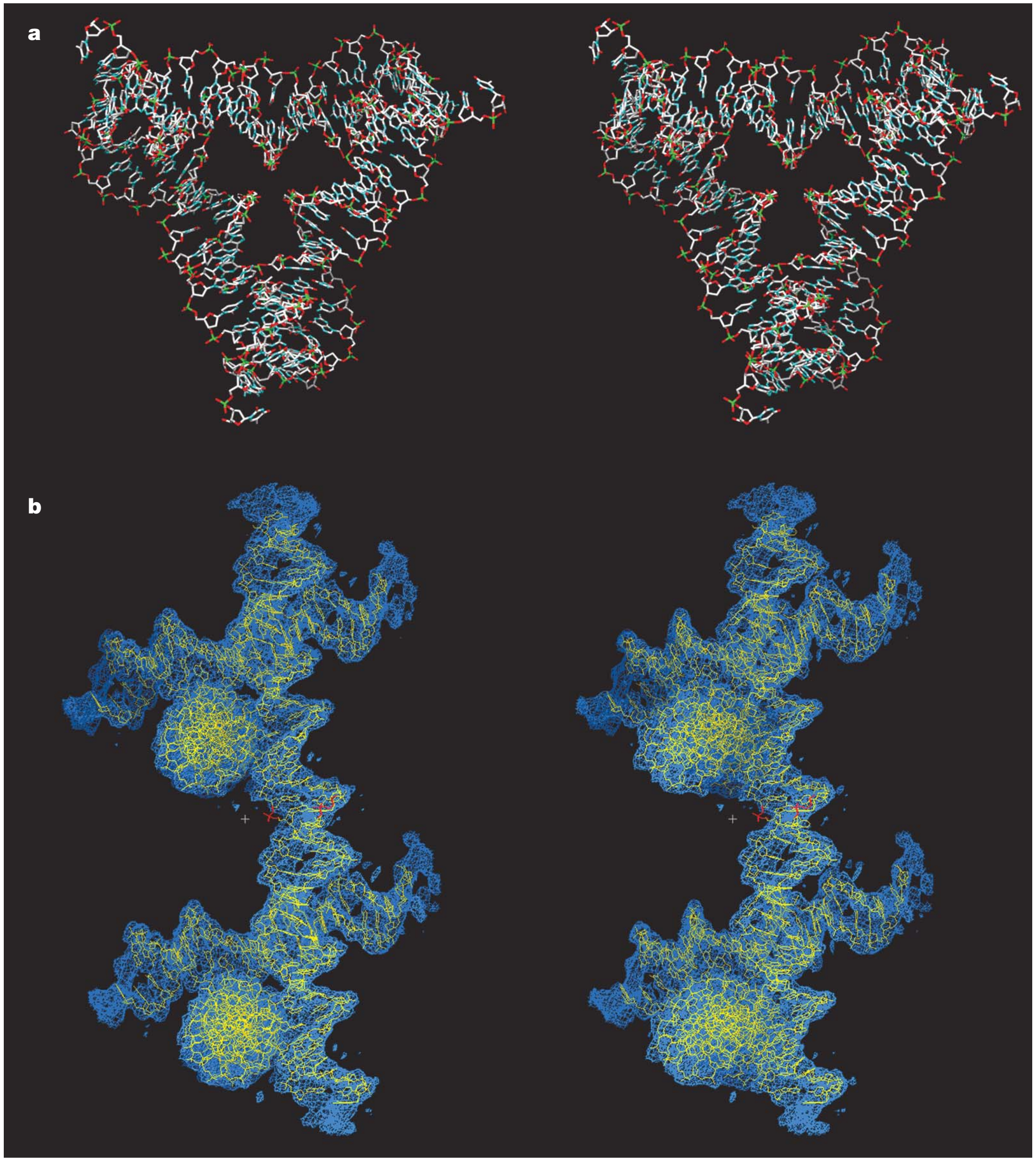


Figure 2 | Views of the tensegrity triangle. **a**, Stereoscopic view of the triangle down its three-fold axis. It is in the same orientation as the schematic in Fig. 1a. The helix on the top edge starts above the mean plane of the molecule at the left and proceeds to the rear as it moves to the right. **b**, Stereoscopic view of two triangles in electron density. This image is perpendicular to an edge of the rhombohedron, showing the connection of two triangles by sticky ends. Sticky ends are magenta for emphasis. Some density features belonging to neighbouring molecules are not depicted.

X-Ray Resolution of Seeman's Tensegrity tiles & 3D lattices

Table 1 | Crystalline tensegrity triangle lattices

Crystal number	Edge length (nucleotide pairs)	Space group	Inter-junction pairs	Rhombohedral cell dimensions	Resolution (Å)	Cross-section (nm^2)	Cavity size (nm^3)
1	21	*R*3	7	$a = 69.2$ Å, $\alpha = 101.4°$	4.0	23	103
2	21	*P*1	7	$a = 68.0$ Å, $\alpha = 102.6°$	5.0	23	101
3	31	*R*3	17	$a = 102.0$ Å, $\alpha = 112.7°$	6.1	62	366
4	31	*P*1	17	$a = 100.9$ Å, $\alpha = 111.6°$	6.3	61	373
5	32	*R*3	18	$a = 103.6$ Å, $\alpha = 113.6°$	6.5	64	367
6	32	*P*1	18	$a = 103.3$ Å, $\alpha = 112.2°$	6.5	64	395
7	42	*R*3	17	$a = 134.9$ Å, $\alpha = 110.9°$	11.0	123	1,104
8	42	*P*1	17	$a = 133.7$ Å, $\alpha = 111.3°$	14.0	120	1,048
9	42	*R*3	28	$a = 134.9$ Å, $\alpha = 117.3°$	10.0	117	643

The cross-sectional area and cavity size are derived from the lattice parameters. Cross-sections and cavity sizes are estimated by subtracting two radii of the double helix (~10 Å) from the unit cell dimensions. The space group indicates whether deliberate three-fold rotational averaging has been performed; it has for those in *R*3, not for those in *P*1. Edge lengths and inter-junction distances (within triangles) are given in nucleotide pairs. Crystal 1 is the work reported here. The structures of crystals 3 and 7 have been determined by molecular replacement; others are in progress.