

## Introduction

Brandeis MRSEC IRG1 envisions to design self-limited structures on length scales many times larger than the building blocks. Nature presents remarkable geometric shapes in the capsids of viruses. During replication inside cells proteins accumulate around the viral genome to create an outer shell which is known as capsid. For example, Cowpea Chlorotic Mottle virus (CCMV) is one of the iconic icosahedral virus whose capsid is made of 180 chemically identical 3 different types of protein subunits.

Cowpea Chlorotic Mottle virus (CCMV)

Scientists discovered a remarkable way to mimic the similar mechanism with the self assembly of DNA origami subunits.. Caspar and Klug elucidated the geometric arrangement of protein subunits on a capsid by Triangulation number (T number).

$$T = h^2 + hk + k^2$$

C. Sigl et al, Nature Materials 20, 1281-1289 (2021)

## Our goal

While smaller viruses are able to spontaneously produce capsid of Icosahedron order, larger viruses require template: scaffolding proteins or inner cores. Simply, the template governs the pathway towards a complex geometry of the capsid.

Our goal is to control the kinetic pathway of template dependent self assembly of DNA origami monomers. We will tune the elastic properties and binding strength of triangular subunits to encapsulate lipid vesicles which will act as template in our system. *Our work aligns with the plan of MRSEC IRG1 to design programmable curvature controlled self-limited assembly.*

Assembly Pathway (Ref: Siyu Li, PNAS, vol 115, no 43 2018)

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## MRSEC annual retreat 2022

### How DNA interacts with lipid bilayer?

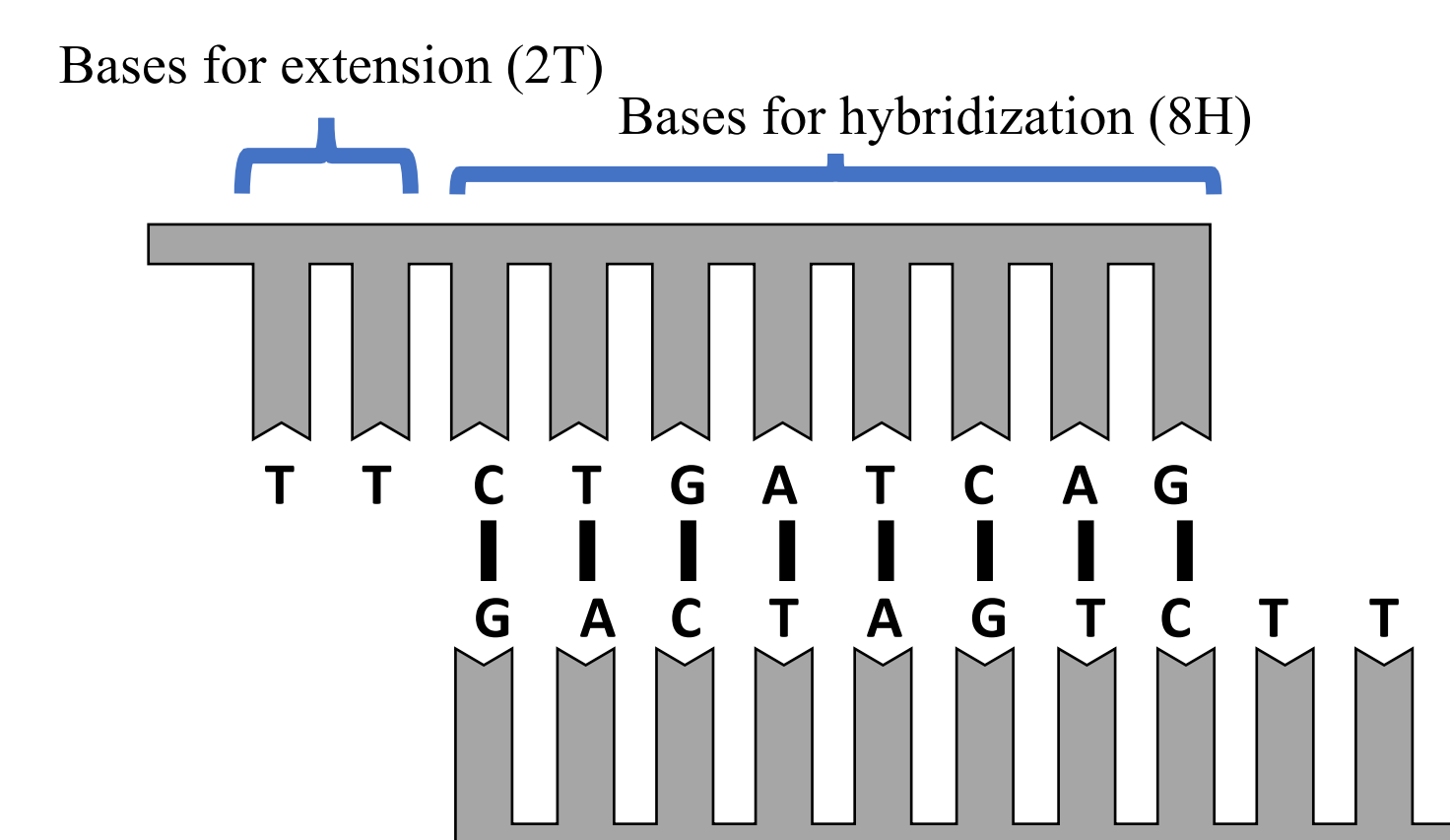
DNA strands are modified with cholesterol. Cholesterol embeds into the lipid membrane due to hydrophobic interaction.

### Our designed triangle

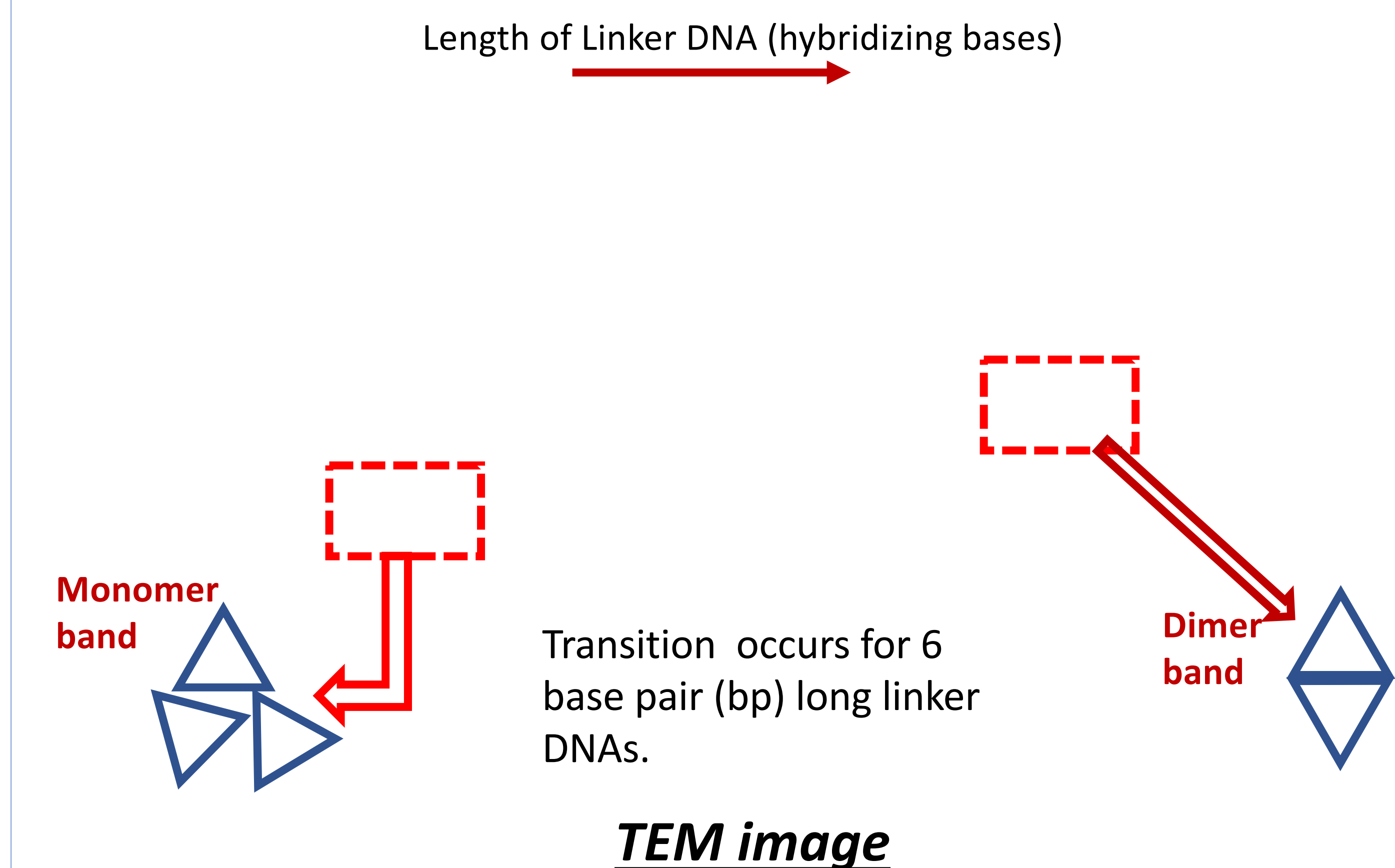
As the dihedral angle can vary, a single species of triangle will be able to form capsids of different sizes from T1 to T9.

### How to modify the stretching and binding strengths between monomers

Bases for extension provides stretching whereas bases for hybridization incorporates binding among monomers



### Transition from monomer to dimers



Triangles with 8 base pair binding strands form dimers when one side is active.

### Future objectives

Our DNA origami triangles show a promising progress towards our goal of forming an icosahedron capsid around a template. However, It is still unknown that what binding strength is adequate to assemble in three dimensions. Also, the assembly kinetics of DNA nano structures on lipid vesicles are not largely realized till date. In future we will systematically modify the monomer design to understand the kinetics and gain more control over the self-assembly pathway.