Exploring the Nano World: Building Nanoscale Structures with Polymer Modeler

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System Model & Algorithm
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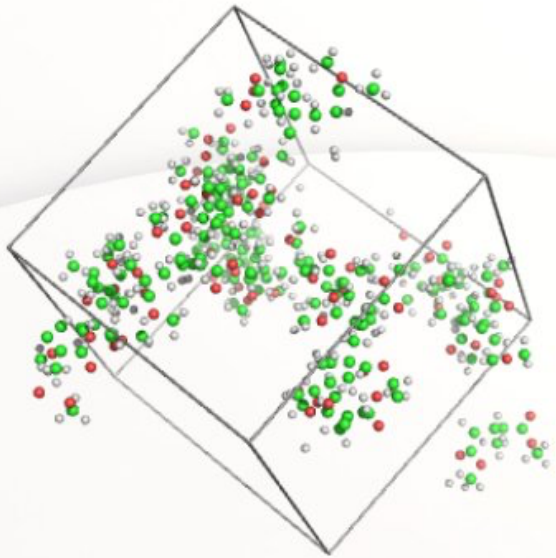
Apple Inc.

Friday, June 9, 2023

2:00 - 3:00 PM EDT



nanoHUB

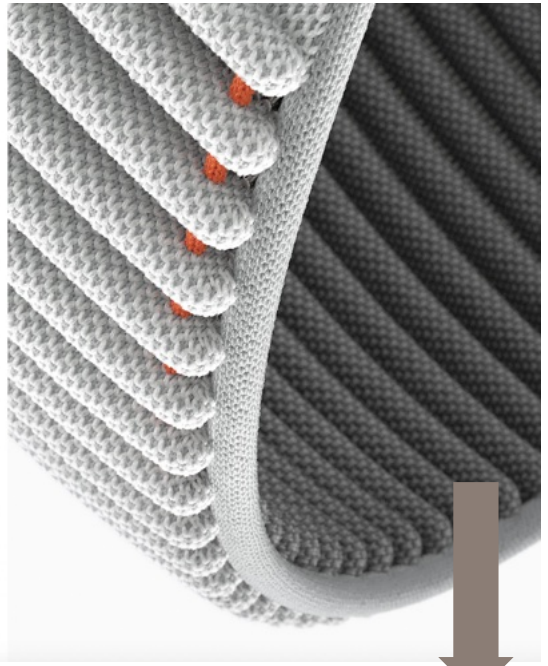
Exploring the Nano World

Crystallization

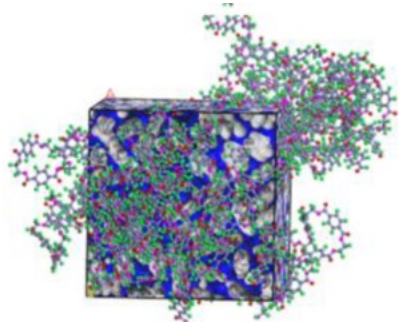
Lightweight Plastic Materials

HDPE (High-density polyethylene)

Transfer fabric materials



60%~70% polyester

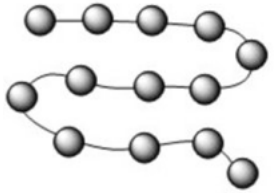


For illustration purpose only, not real material breakdown, Google images

What are Polymer Materials?

Polymers are materials made of long, repeating chains of molecules.

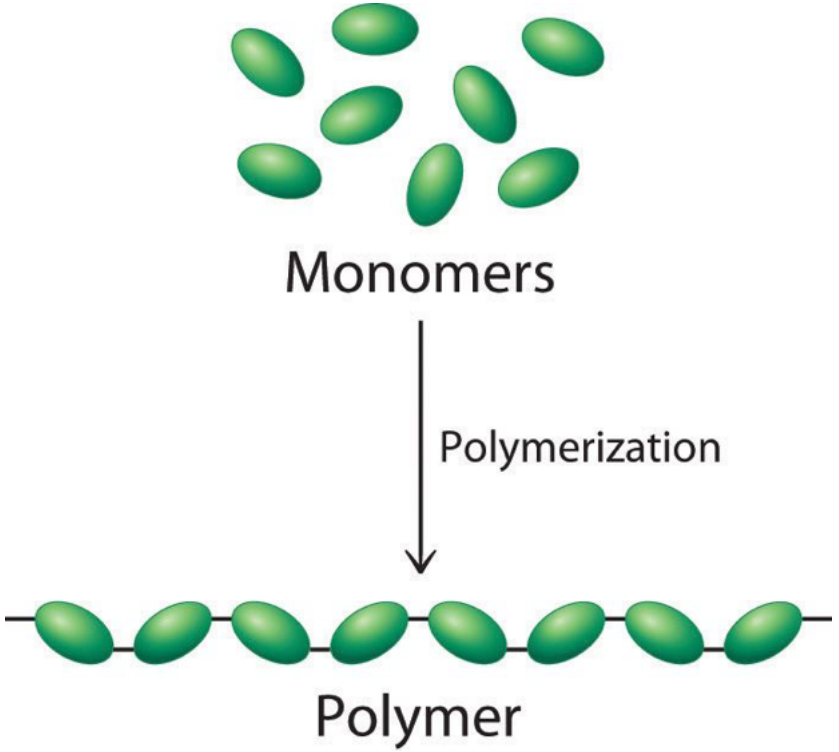
Thermoplastic



Thermoplastics are materials which become soft when heated and hard when cooled.

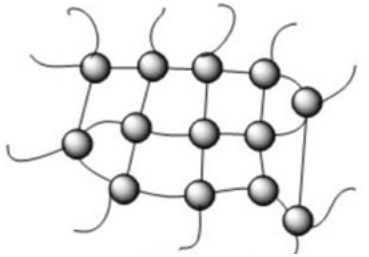
Polyethylene(PE)

Polyvinyl chloride (PVC)



(Image credit: LibreTexts)

Thermoset



Thermosets, materials that are irreversibly hardened by curing from a soft solid or viscous liquid prepolymer or resin.

Fiber-reinforced materials

P.R.O. Transfer fabric

Melamine-resin plate

Google images: *newairplane.com, wikipedia.org*

Polymer Science Paradigm

Properties

Structure

Processing

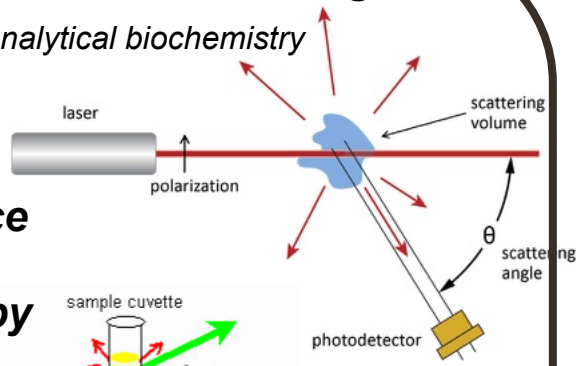
Polymer Science

Design

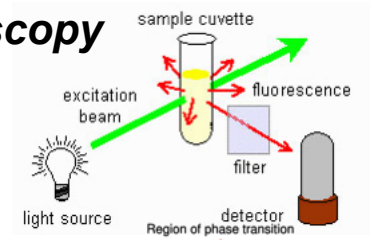
Experimental

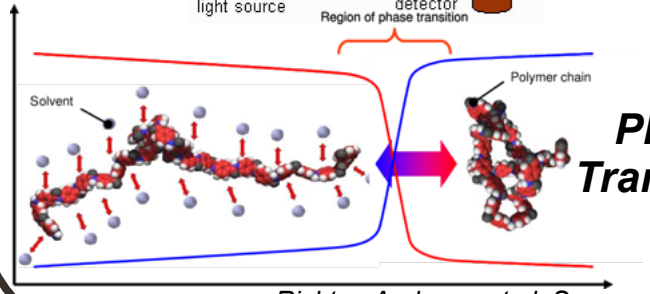
Light & Neutron Scattering

Minton, Allen P. Analytical biochemistry 2016



Fluorescence & NMR Spectroscopy





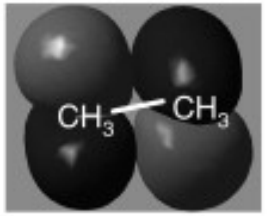
Phase Transition

Richter, Andreas, et al. Sensors 2008

Simulation

Quantum Models

$$H(t)\left|\Psi(t)>=ih\frac{d}{dt}\right|\Psi(t)>$$

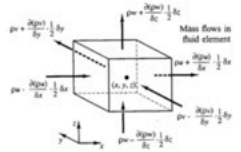


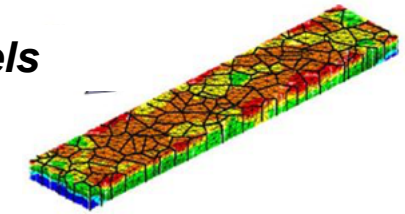
Classical Models

$$\vec{F}=\mathrm{m}\vec{a}=-\nabla_r V(r)$$

Alemán, Carlos, et al. Journal of Molecular Structure 2009

Continuum Models

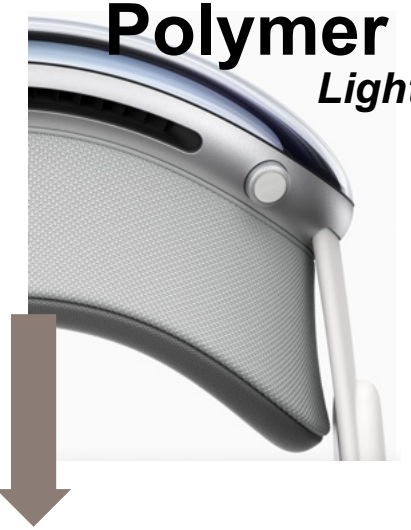




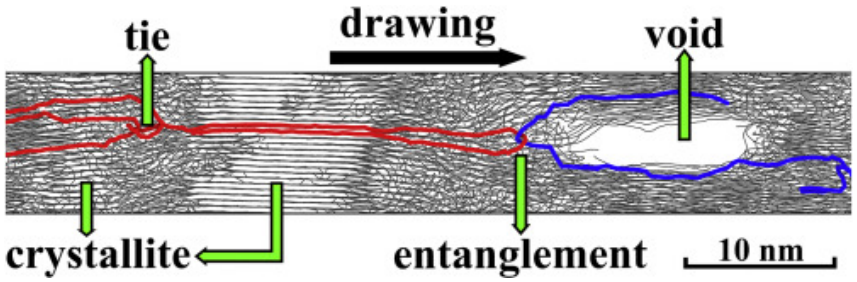
Google images: *slideplayer.com, chromedia.org,*

Polymer Modeler Advanced Case Study: Polyethylene Crystallization

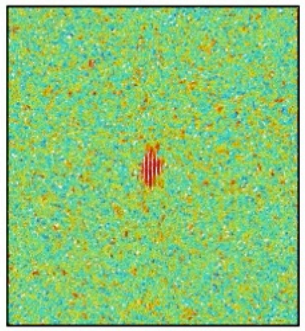
Lightweight Plastic Materials

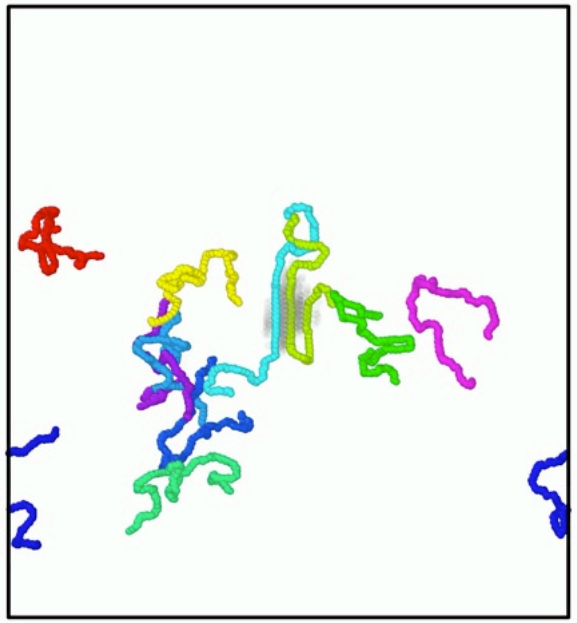


HDPE (High-density polyethylene)



Tm ~ 137°C/278F





137°C/278F K – 150 ns

Shen, et al. Physical Review Letters, 2020.

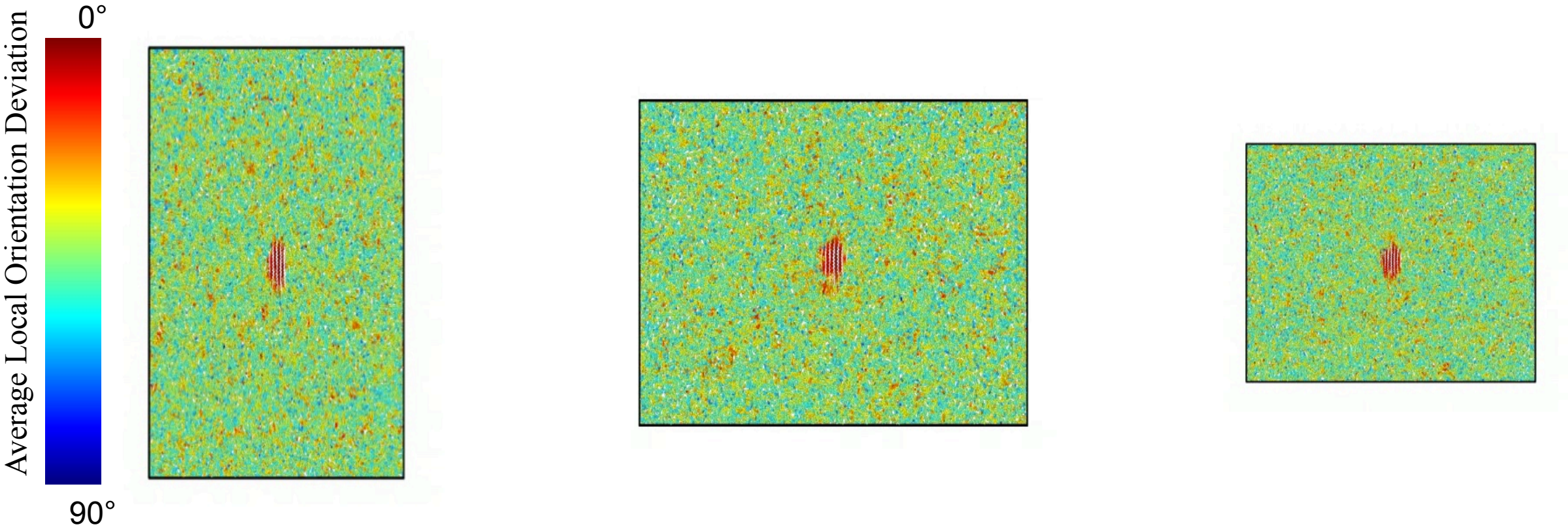
Polymer Modeler Advanced Case Study: Polyethylene Crystallization

77°C/152F – 100 ns
Induced Nucleation Starts 5 ns

97°C/188F – 100 ns
Induced Nucleation Starts 14 ns

117°C/224F – 100 ns
Induced Nucleation Starts 35 ns

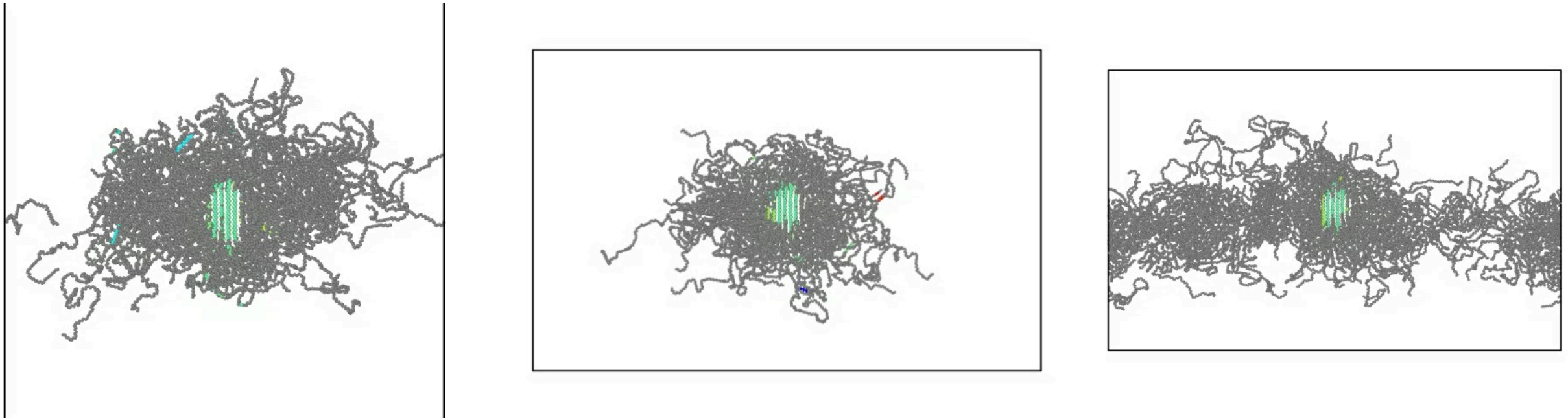
Temperature



Shen, et al. Physical Review Letters, 2020.

Polymer Modeler Advanced Case Study: Polyethylene Crystallization

77°C/152F – 100 ns **97°C/188F – 100 ns** **117°C/224F – 100 ns**



Changing of the shape of the molecules observed

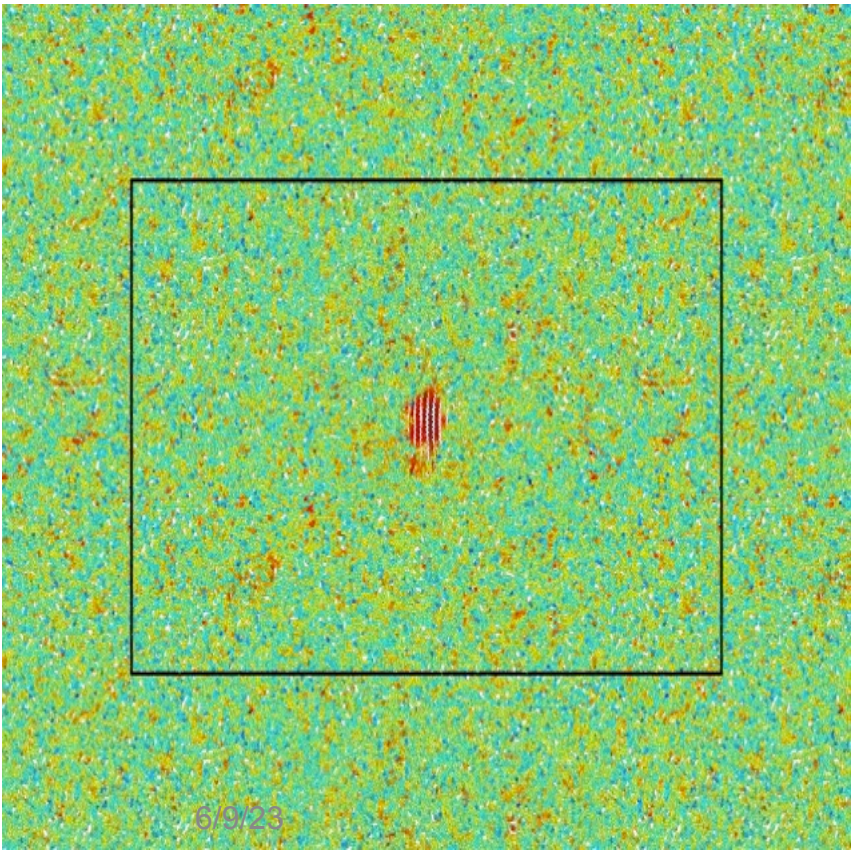
Shen, et al. Physical Review Letters, 2020.

Polymer Modeler Advanced Case Study: Polyethylene Crystallization

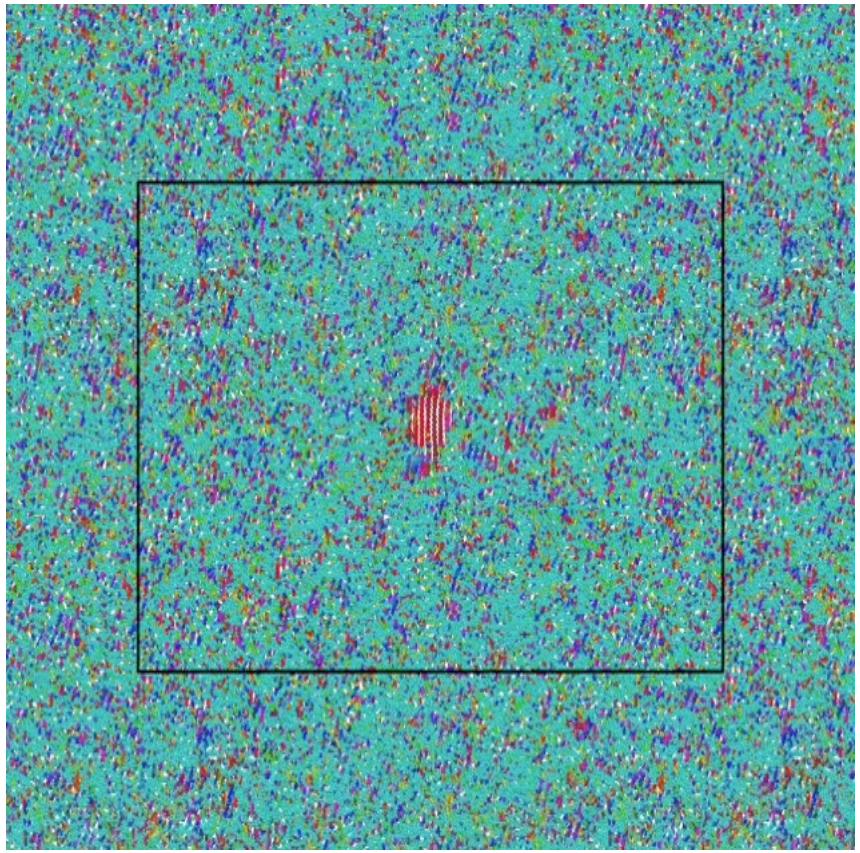
0° 90°

-40° 40°

Local Alignment Map



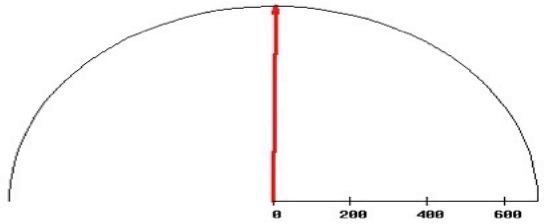
Local Orientation Map



Cluster Orientation

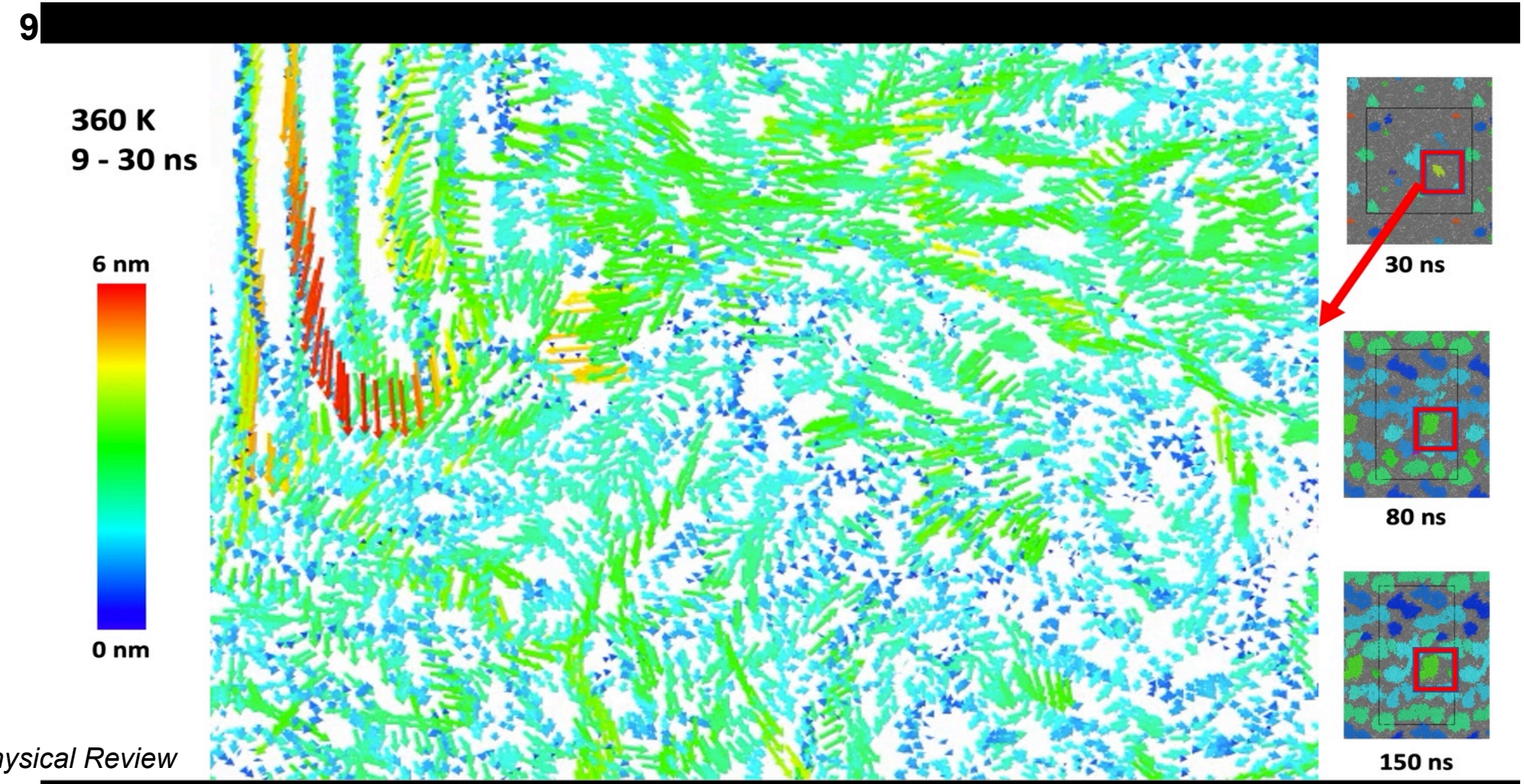
97°C/188F – 100 ns

Dynamic Axis



Shen, et al. Physical Review Letters, 2020.

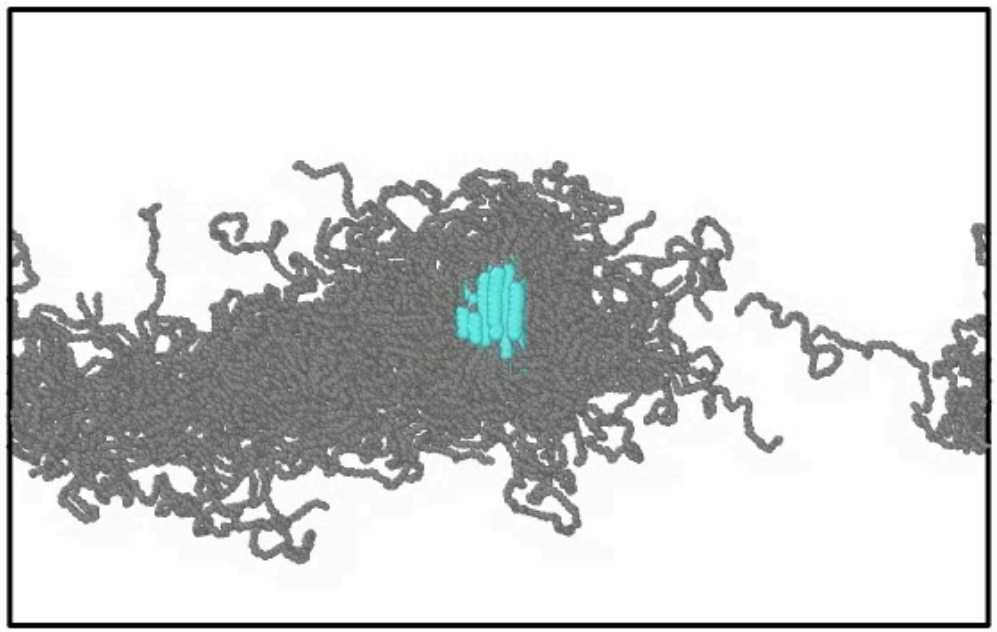
Polymer Modeler Advanced Case Study: Polyethylene Crystallization

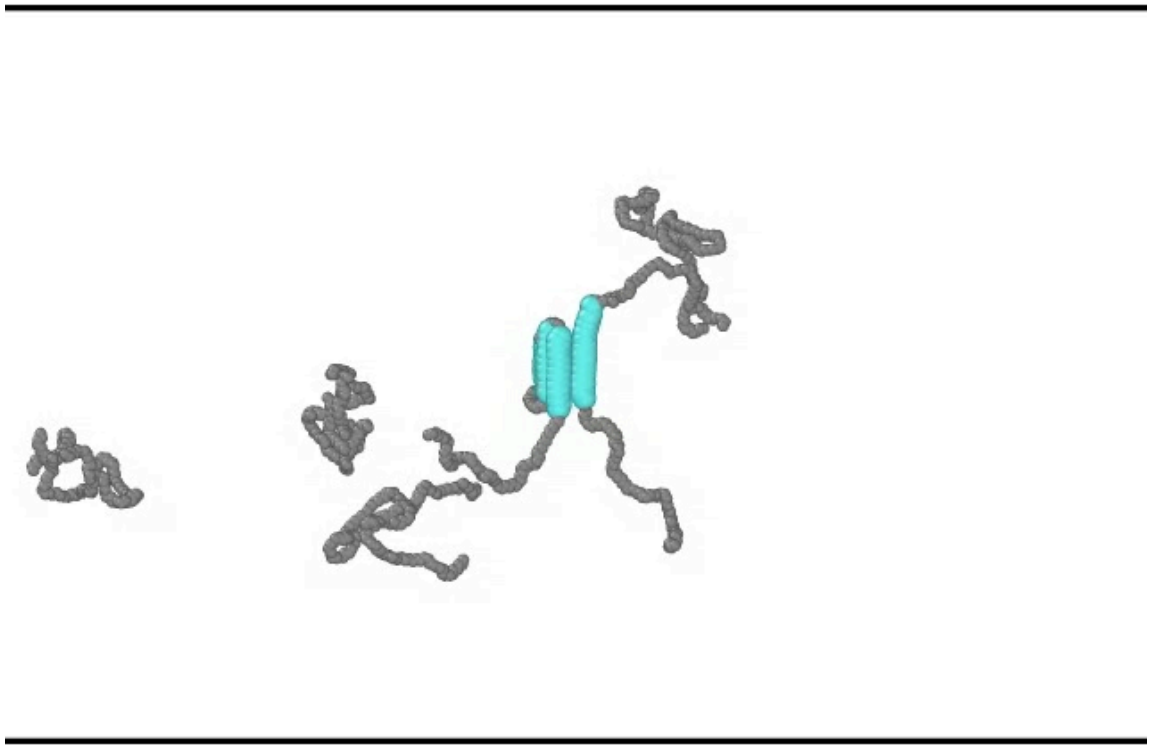


Shen, et al. Physical Review Letters, 2020.

Polymer Modeler Advanced Case Study: Polyethylene Crystallization

360 K – 191 ns





Shen, et al. Physical Review Letters, 2020.

Crystal Structures Generation

- Chain Helix
  - Input

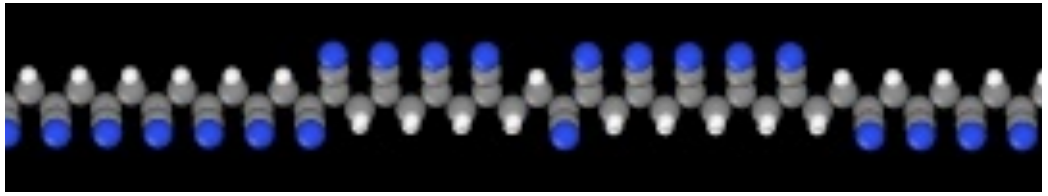
Monomer info:

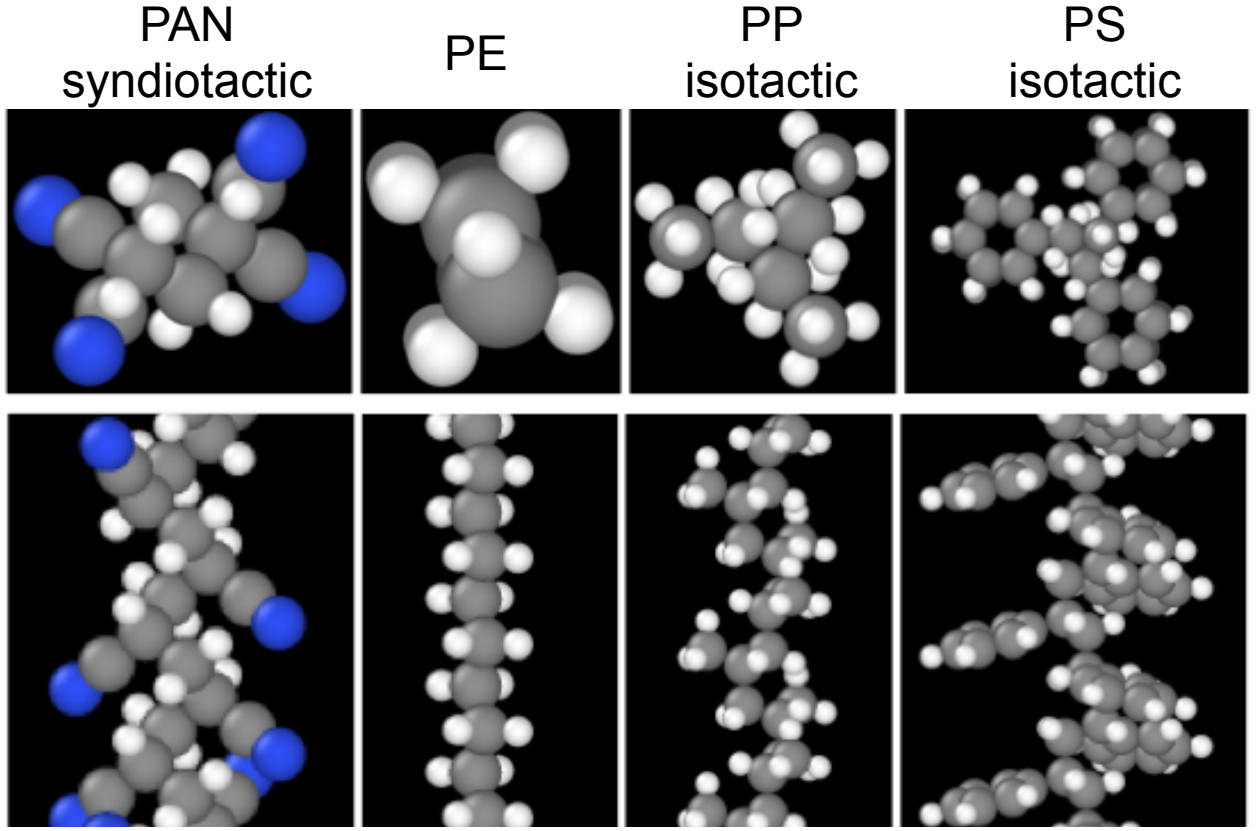
Monomer configuration (.pdb, .xyz, .zm);
Indices of backbone atoms & side atoms

Chain configuration:

Tacticity (isotactic, syndiotactic, atactic)
Helicity (helix 2*3/1, 2*2/1, 2*1/1 – planar zigzag)
Chiriality (left, right)
Defect ratio of head-to-head, tail-to-tail connections

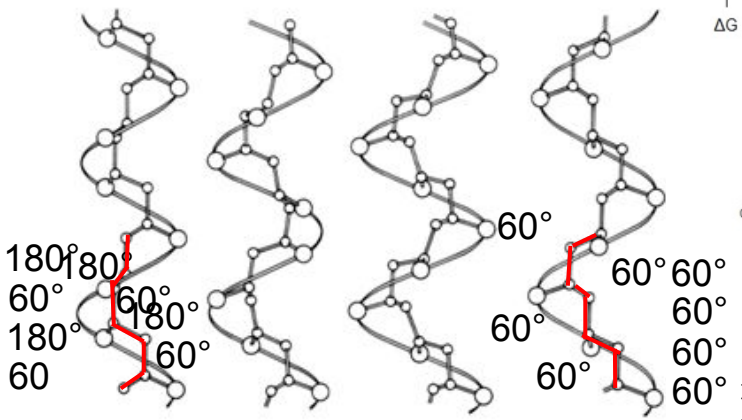
Example of isotactic PAN with 10% defects





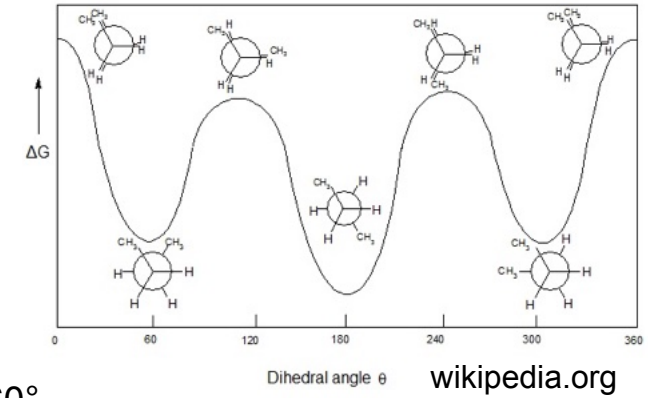
Polymer Stereoregularity

How these helix form?

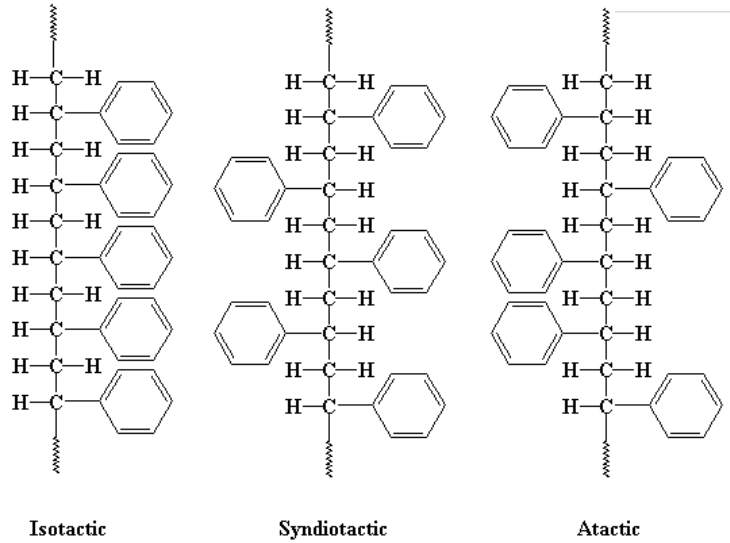


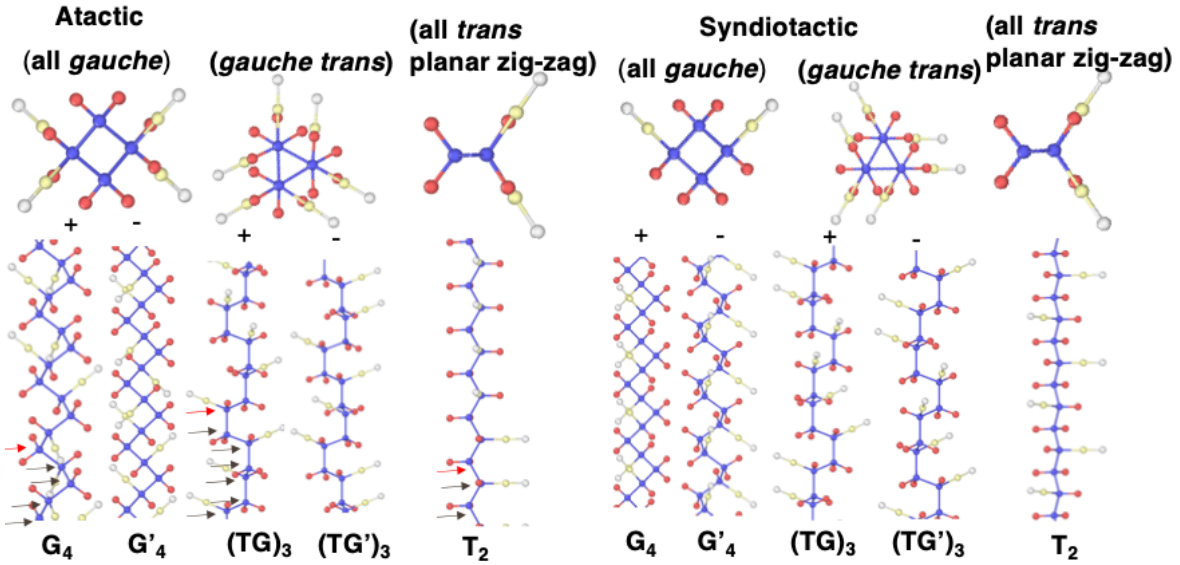
Helix 2*3/1

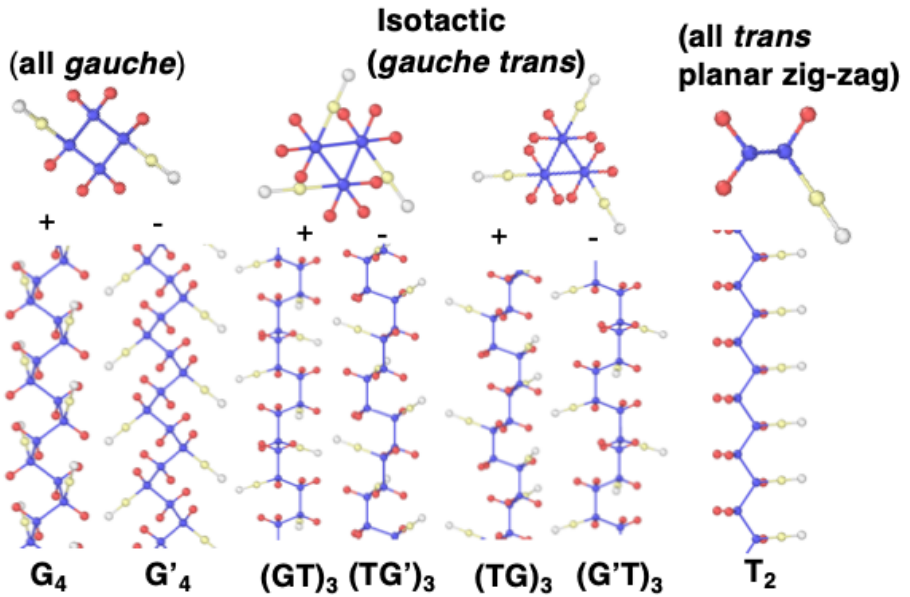
Helix 2*2/1



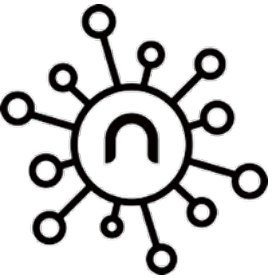
wikipedia.org

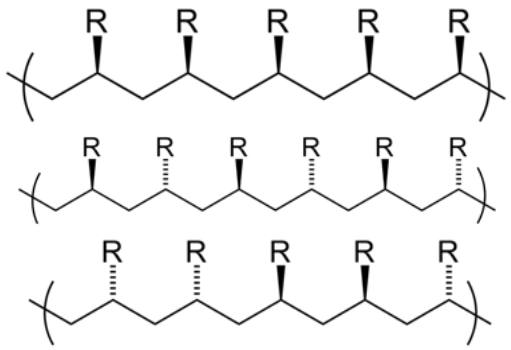


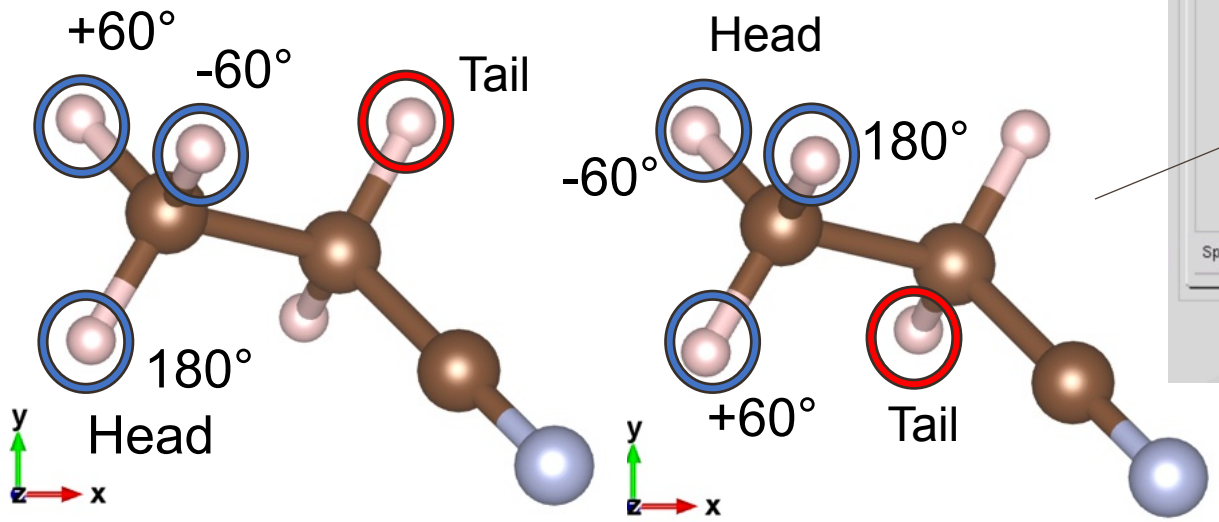


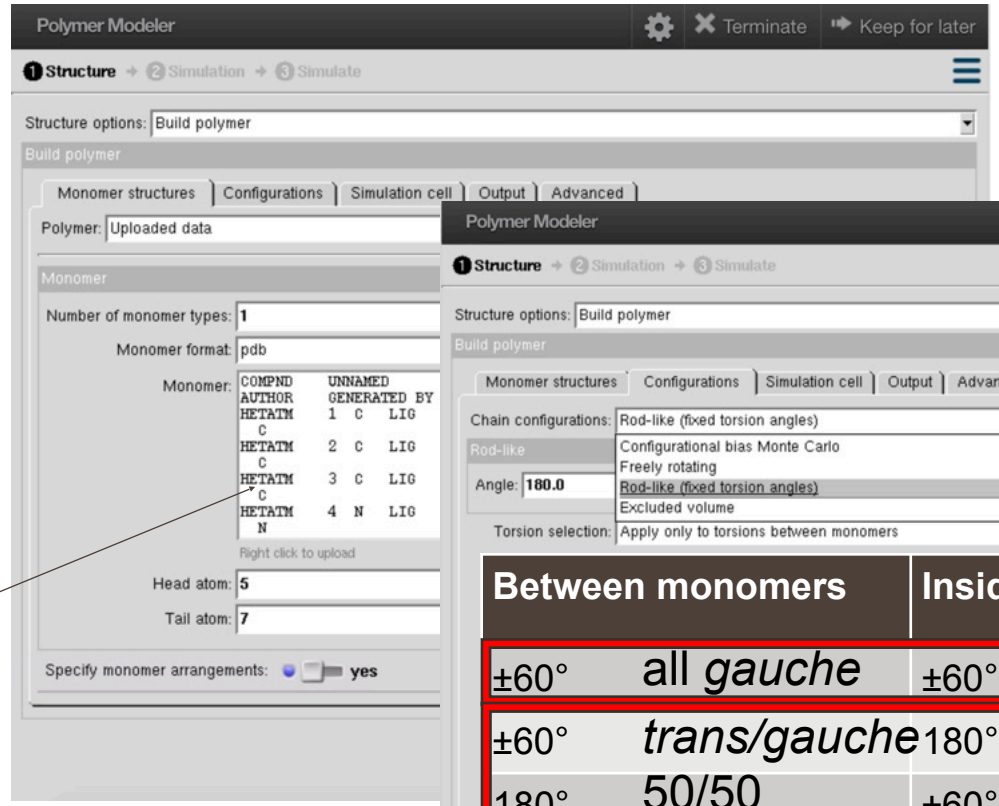


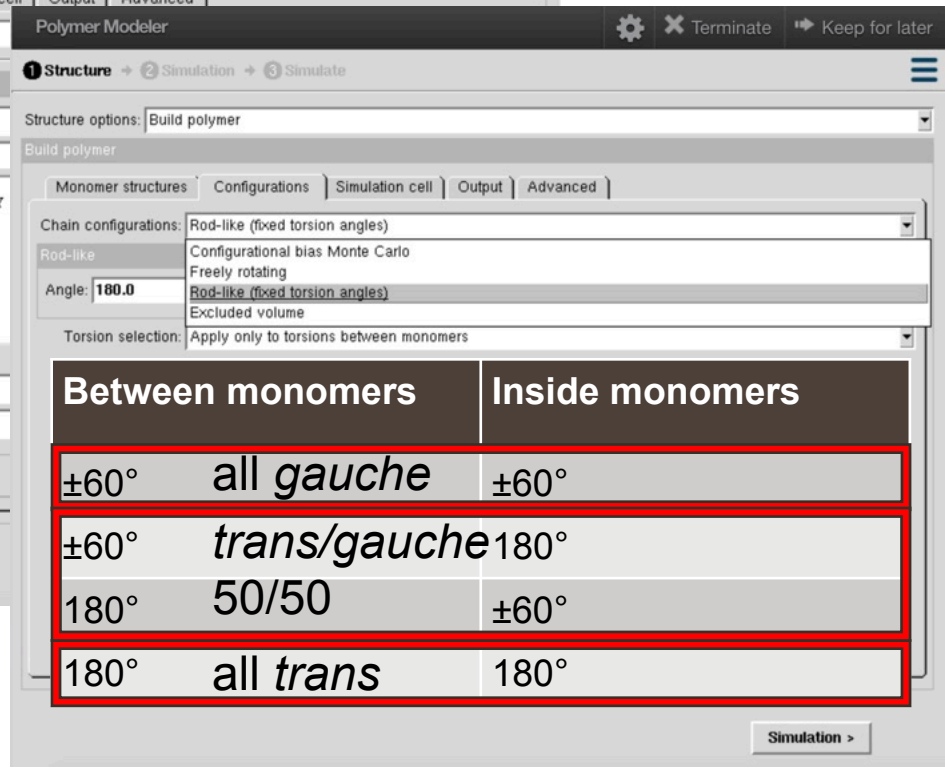
Generating rod-like PAN chains with *trans-gauche* conformations











Between monomers		Inside monomers
±60°	all *gauche*	±60°
±60°	*trans/gauche*	180°
180°	50/50	±60°
180°	all *trans*	180°

THANK YOU