Ph.D. Dissertation Defense

Stress-strain Response of High-performance Crystalline Aromatic-aliphatic Polyamides

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October 24, 2022

Film

www.testresources.net

Foam

www.familyhandyman.com

Fiber

www.made-in-china.com

Frame

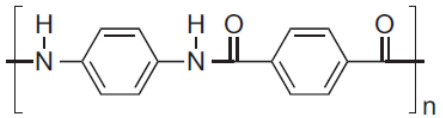
www.microsoft.com

Rubber

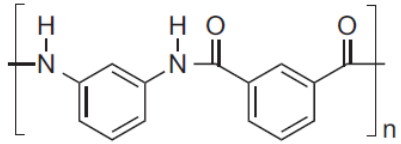
www.tirerack.com

- Excellent **mechanical** strength per unit weight,
- High **thermal** stability (continuous use temperatures above 150 °C, combined with low flammability),
- **Chemical** resistance (also at elevated temperatures)
- **Electrical** properties (e.g., as insulators)

Aromatic polyamide

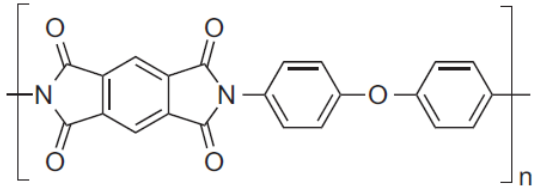


Kevlar

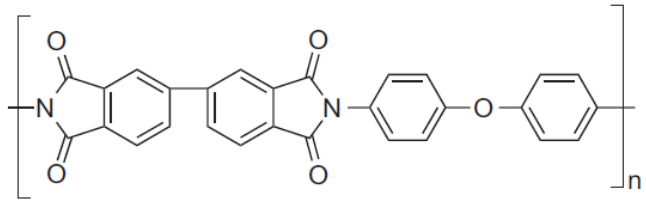


Nomex

Aromatic polyimide

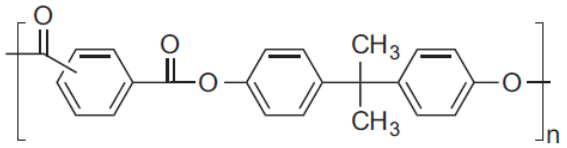


Kapton



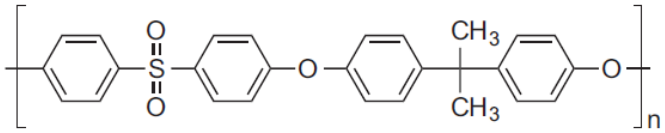
Upilex R

Aromatic polyester



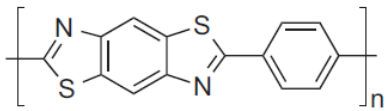
U-polymer

Aromatic polysulfone



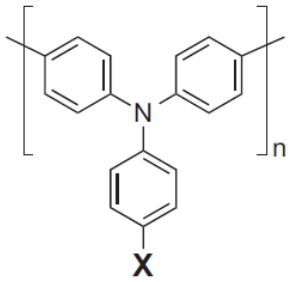
PST

Aromatic heterocyclic polymer



PBT

Aromatic polytriphenylamine



X

Polymer Journal 48.2 (2016): 117-138.

- Aromatic polyamides (aramids), such as poly(*p*-phenylene terephthalamide) (PPTA), which is also trademarked as Kevlar® and Twaron®
- Excellent thermal and oxidative stability, high mechanical strength, low flammability and good chemical and radiation resistance.

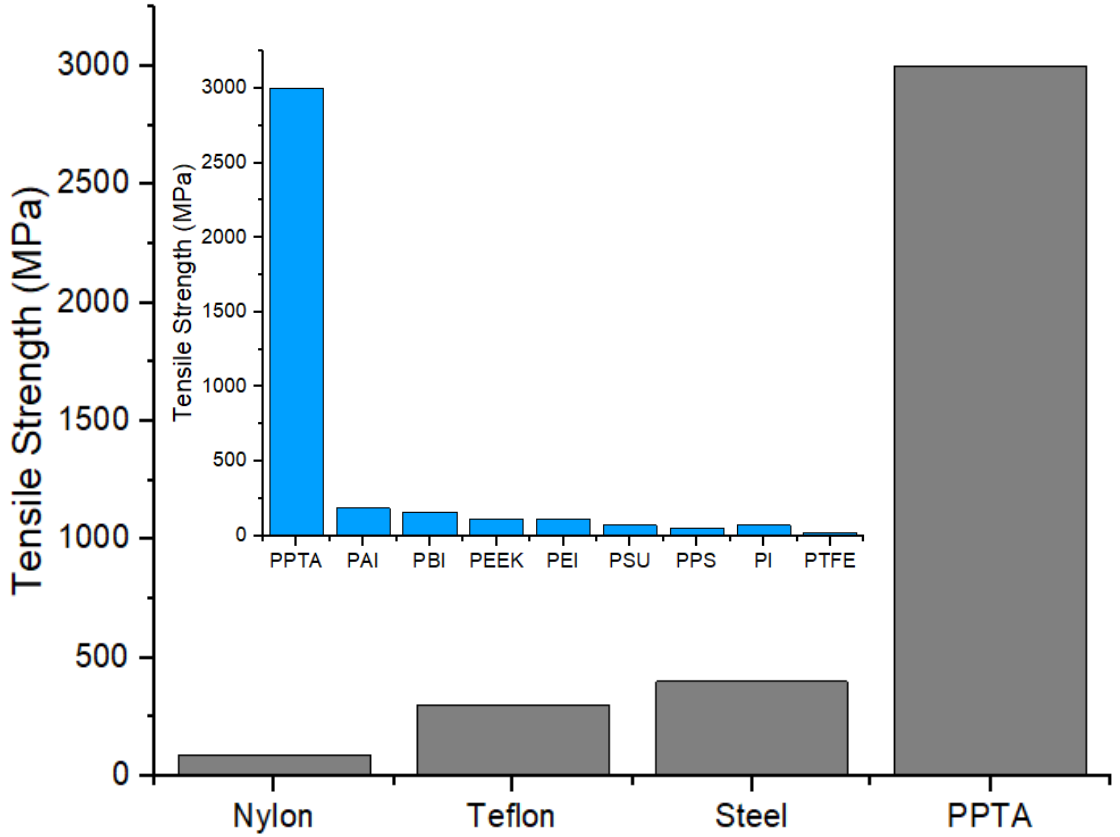
www.walmart.com

www.il.ngb.army.mil

www.superleggera.com.au

en.wiktionary.org

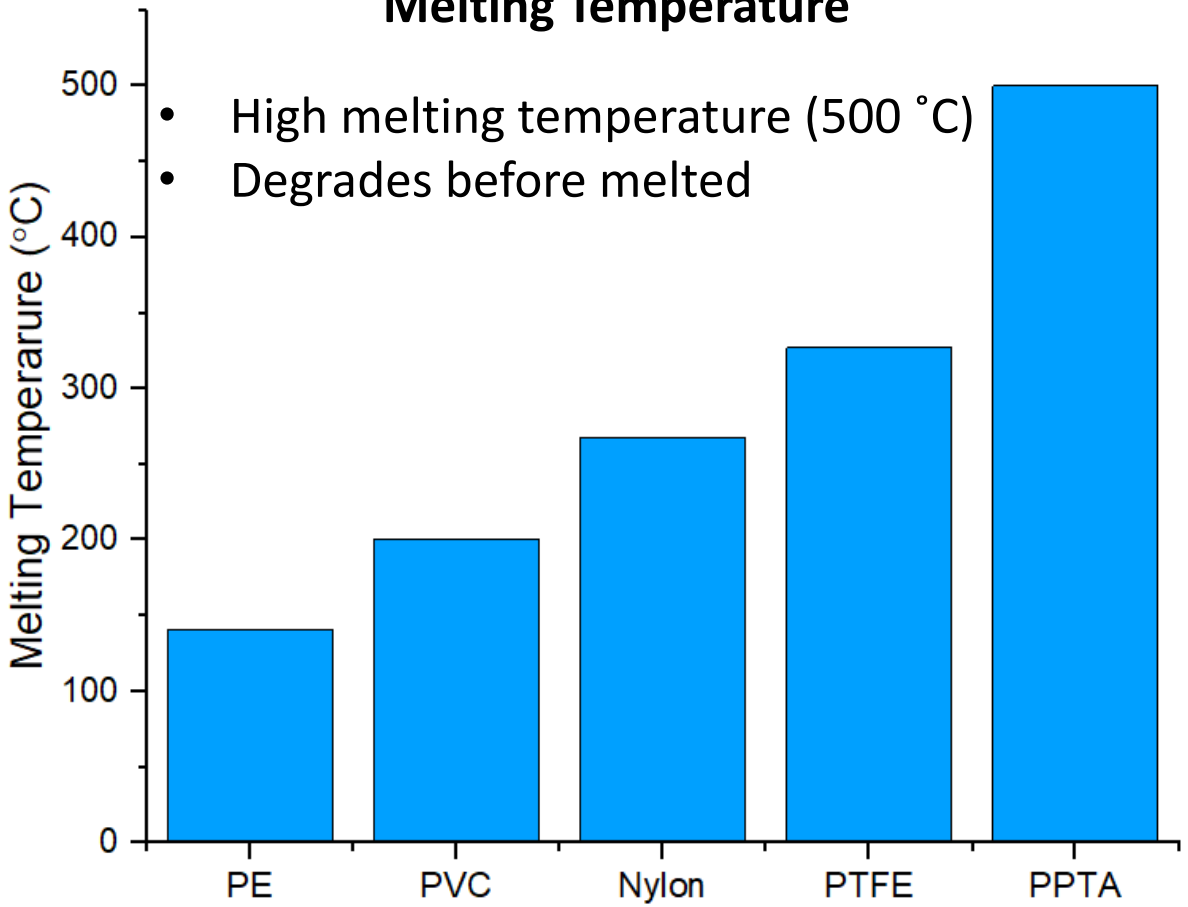
- Tensile strength of PPTA is much higher than other commonly seen polymers and even 5 times higher than steel



- Melt processing and solution processing
- Hard to process (injection, extrusion, and 3D printing)

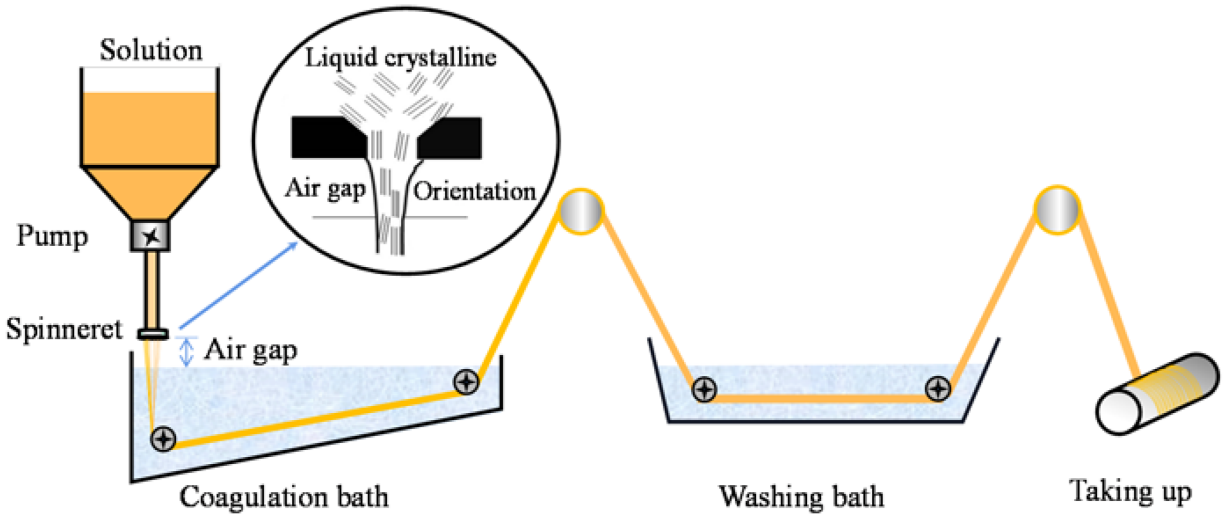
Melting Temperature

- High melting temperature (500 ˚C)
- Degrades before melted



Solubility

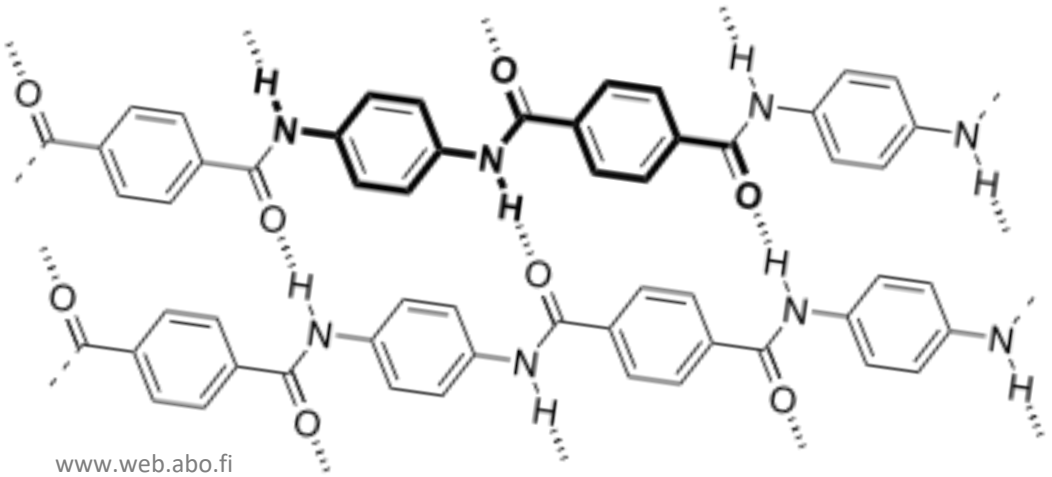
- Only soluble in strong acids such as sulfuric acid (H_2SO_4), which is not economically or environmentally friendly



Polymers 12.5 (2020): 1206.

Reasons for high melting temperature:

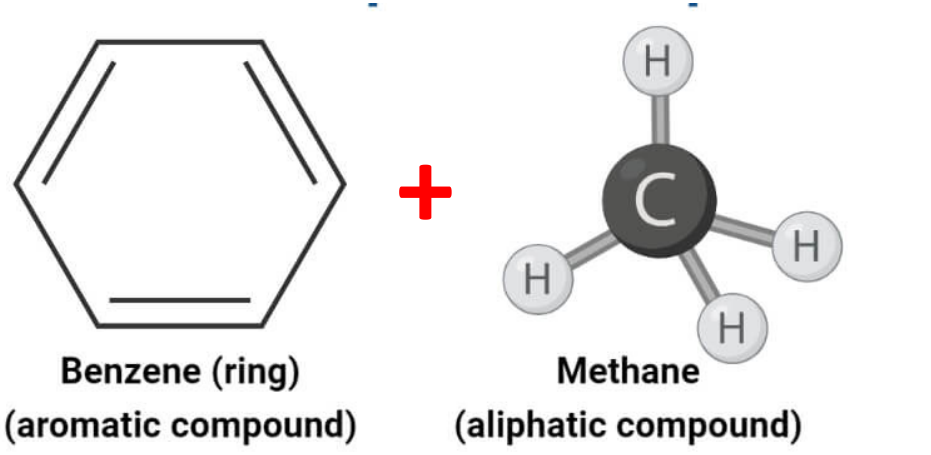
- rigid structure of aromatic moieties
- low flexibility of the chains (no rotation)
- strong intermolecular interactions

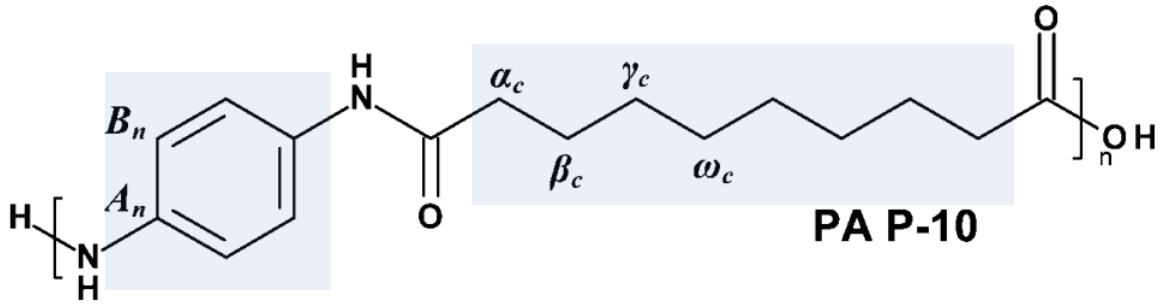


www.web.abo.fi

Solution:

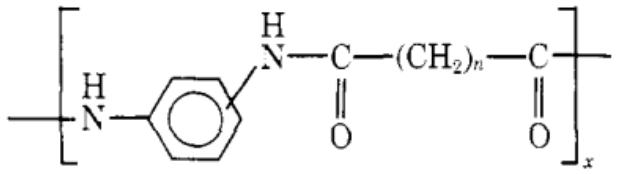
- Increase flexibility of the structure
  - Introducing flexible aliphatic compound to be aromatic-aliphatic polyamide
  - PAPX, X is depending on how many methylene units are included

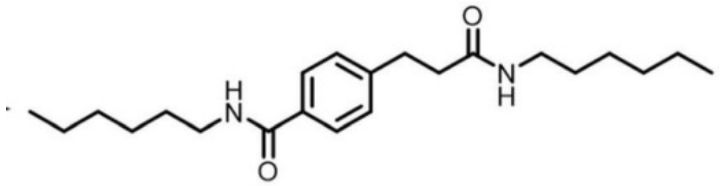


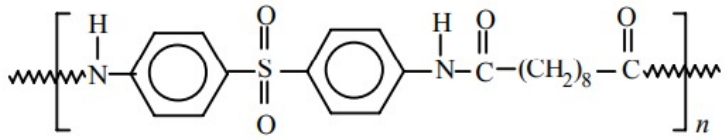


Macromolecules 49.3 (2016): 950-962.

Researchers synthesized polyamides containing various aromatic and aliphatic compounds.[1,2,3]
It was found that the melting temperature increases with increasing aromaticity but decreases with increasing length of aliphatic chain. [1,2,3]







However, it was also found that the introduction of flexible aliphatic compounds will cause a reduction in the thermal and mechanical properties (tensile strength, ultimate strain, and Young's modulus). [4,5]

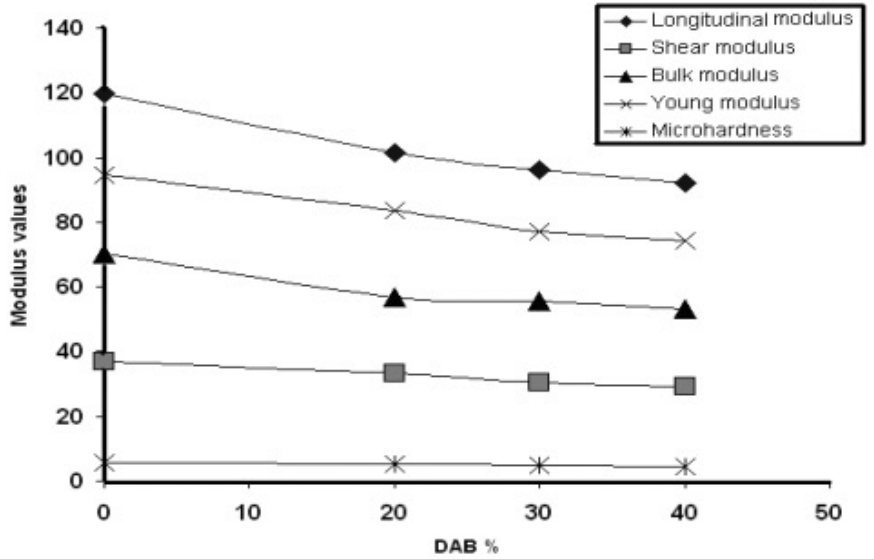
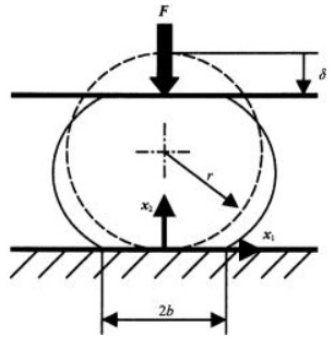


Figure 11. Plot of Modulus values vs. DAB %

[1] *Macromolecules* 8.2 (1975): 104-111.
[2] *Journal of Polymer Science: Polymer Physics Edition* 15.3 (1977): 587-590.
[3] *Polymer Chemistry* 12.16 (2021): 2379-2388.
[4] *Advances in Polymer Technology* 29.4 (2010): 300-308.
[5] *American Journal of Polymer Science* 2.1 (2012): 7-13.

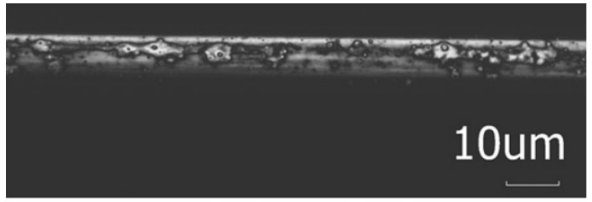
1. Difficult, time-consuming, and requiring sensitive equipment to experimentally capture minor changes in the molecular structure.

2. Experimentally difficult to apply tensile stress on crystal polymers in the directions that transverse to the chain direction

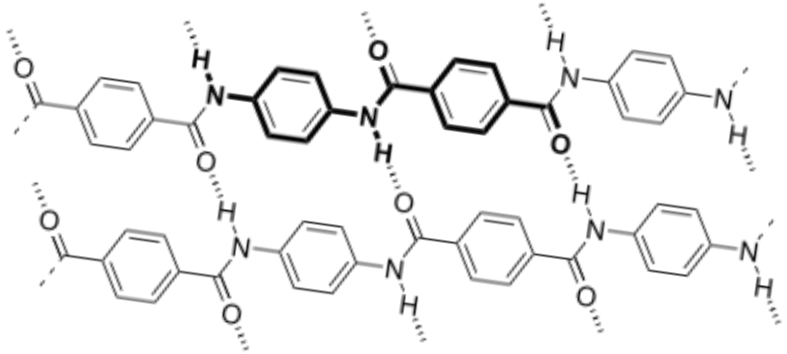


Transverse compression

3. Challenging to obtain large well aligned single crystal and the morphology of the polymers is complicated (e.g., non-crystalline regions and defects)

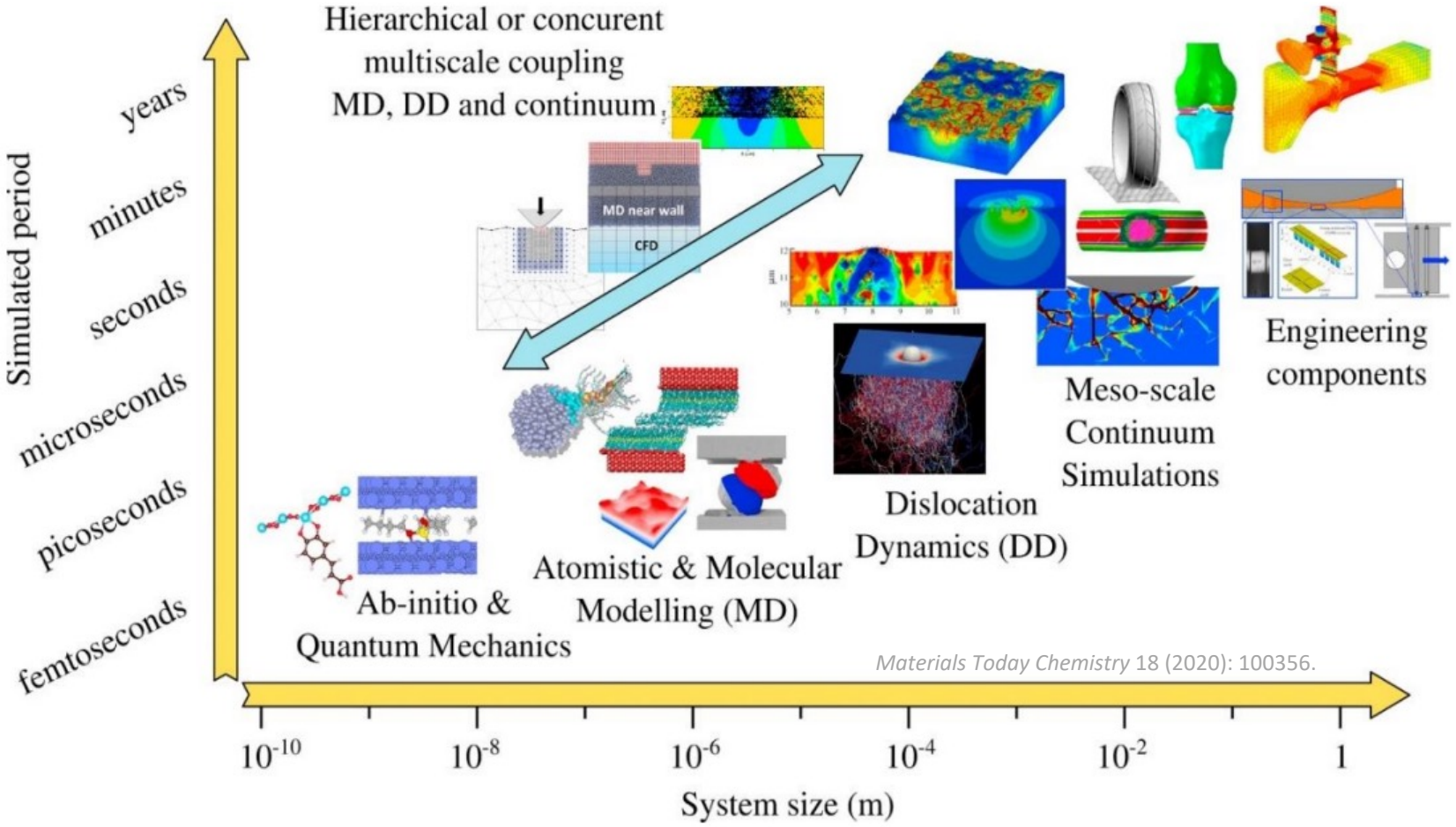


4. Hard to distinguish the relative contributions of intramolecular (e.g., covalent bonds) interactions and intermolecular interactions (e.g., H-bonding and pi-stacking) to bulk mechanical properties.



Textile Research Journal 87.8 (2017): 984-1010.
Polymer Engineering & Science 34.2 (1994): 141-152.
US Army Research Laboratory Aberdeen Proving Ground United States, 2018.
Polymer 22.7 (1981): 960-965.
Journal of materials science 9.11 (1974): 1809-1814.
Journal of Materials Science 35.3 (2000): 573-581.

Time scale vs. Length scale of computational methods



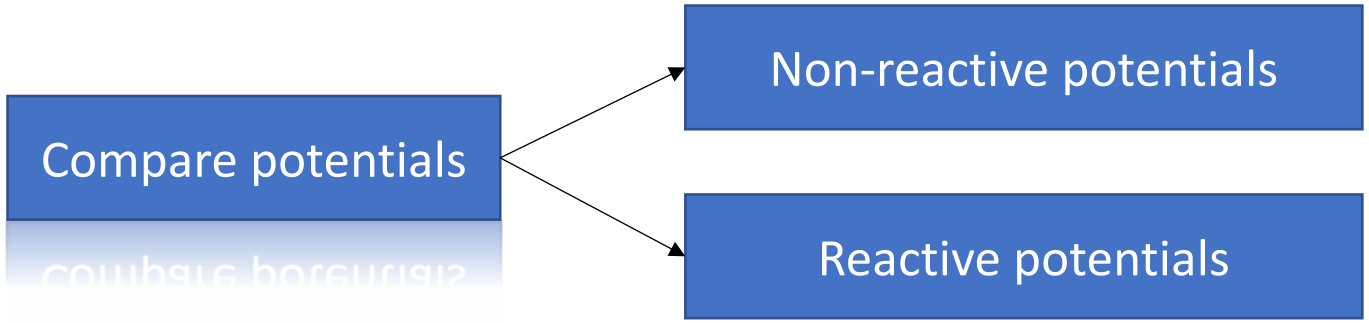
Materials Today Chemistry 18 (2020): 100356.

- MD simulations have been successfully applied to study aromatic-aliphatic polyamide crystals, including the role of aliphatic and aromatic groups on intermolecular interactions, free volume, and glass transition temperature [1, 2], the origin of melting, and the influence of methylene segments on crystal packing and chain conformation [3].

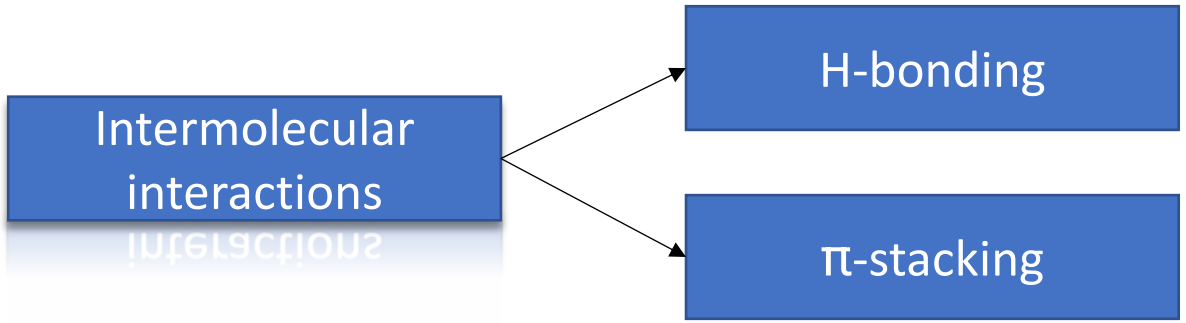
[1] *Polymer* 81 (2015): 50-61.
[2] *Dynamic Behavior of Materials, Volume 1*. Springer, Cham, 2014. 187-193.
[3] *Macromolecules* 49.3 (2016): 950-962.

Limitations of Previous Sim. Studies

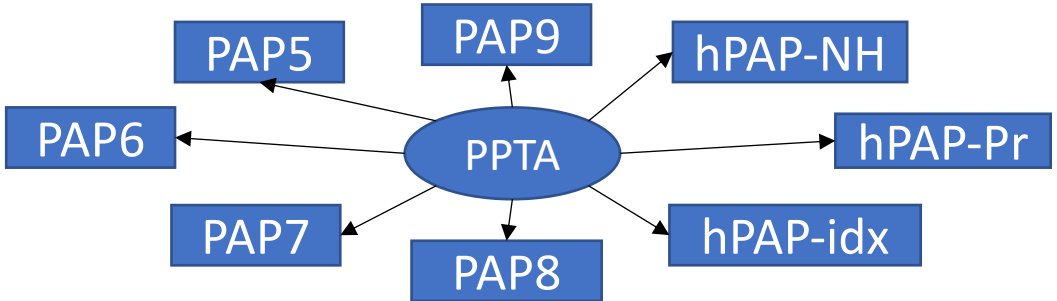
- No comparison of a comprehensive set of potentials, including multiple reactive and non-reactive models



- No evaluation of the ability to model H-bonding and π-stacking patterns



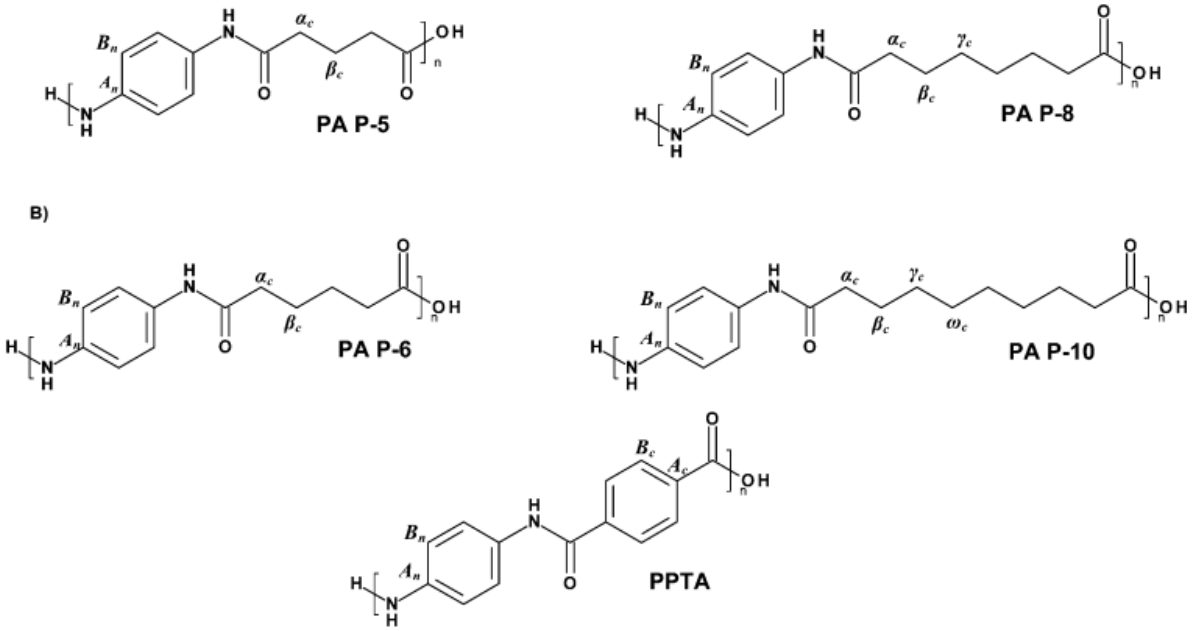
- No generalizability assessed by evaluating homologous material systems

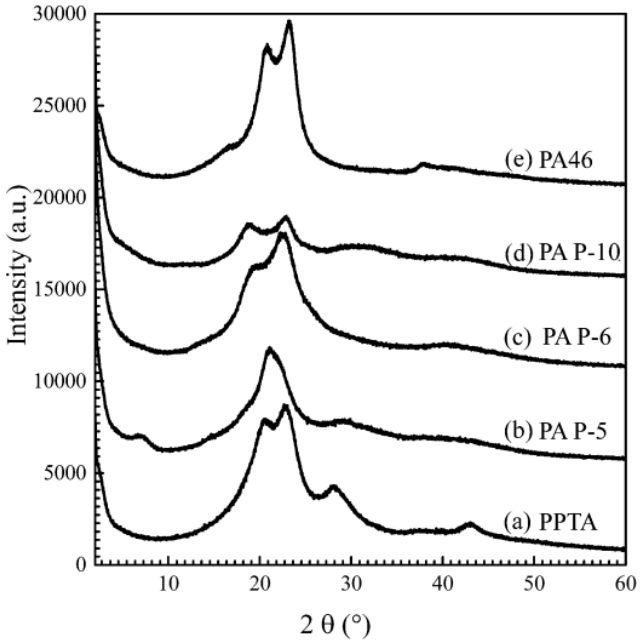


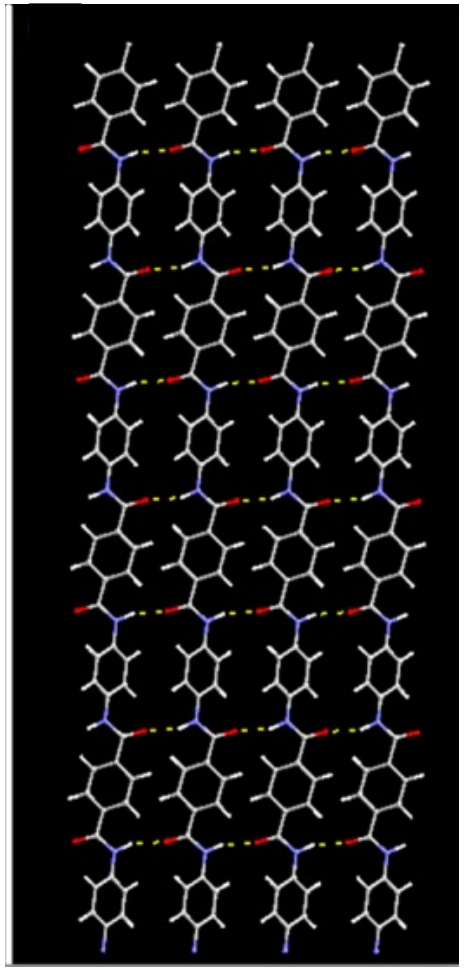
[1] *Journal of Materials Engineering and Performance* 20 (2011), pp. 1401-1413
[2] *Journal of Materials Science* 46.14 (2011), pp. 4787-4802.
[3] *Journal of Materials Engineering and Performance* 22.3 (2013), pp. 681695.
[4] *Advances in Materials Science and Engineering* 2013 (2013), pp. 115.
[5] *Journal of Materials Engineering and Performance* 22.11 (2013), pp. 3269-3287.
[6] *Journal of Materials Science* 49.24 (2014), pp. 82728293.
[7] *Polymer* 114 (2017): 329-347.

- Deshmukh et al. studied the conformational and structural changes with increasing methylene segment length in aromatic–aliphatic polyamides
- They found that the melting temperature decreases with increasing methylene length

polymer	symmetry	unit cell parameters					
		a (nm)	b (nm)	c (nm)	α (deg)	β (deg)	γ (deg)
PPTA (modification I)	$P11n$	0.787	0.518	1.290			90
PA P-5	$P1$ (pseudo $P1a1$)	0.850	0.470	2.480	90	85	90
PA P-6	$P1$	0.540	0.700	2.800	38.5	77	63.5
PA P-10	$P1$	0.504	0.549	3.807	47.1	81.9	93.6
PA 6,10 (α form)	$P1$	0.495	0.540	2.240	49.0	76.5	63.5



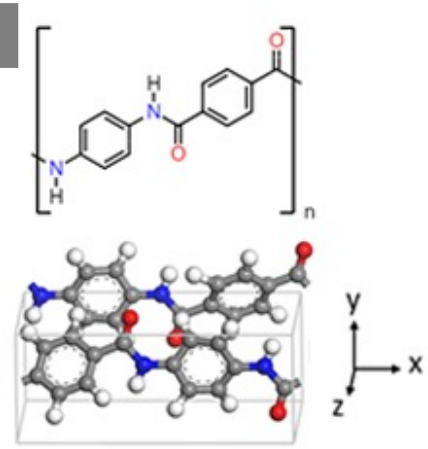




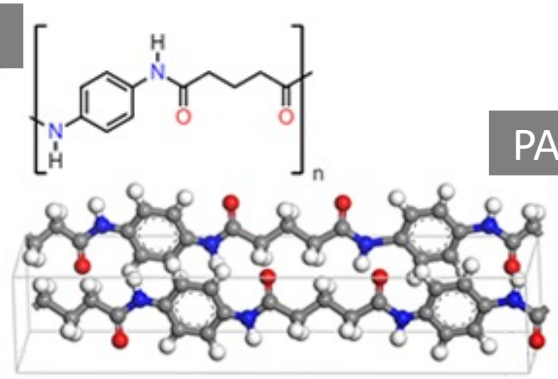
Macromolecules 49.3 (2016): 950-962.

- PAP5 to PAP8 are four example aromatic-aliphatic polyamides
- They all have aromatic and amide groups
- The difference among them is the number of carbons between the aromatic rings

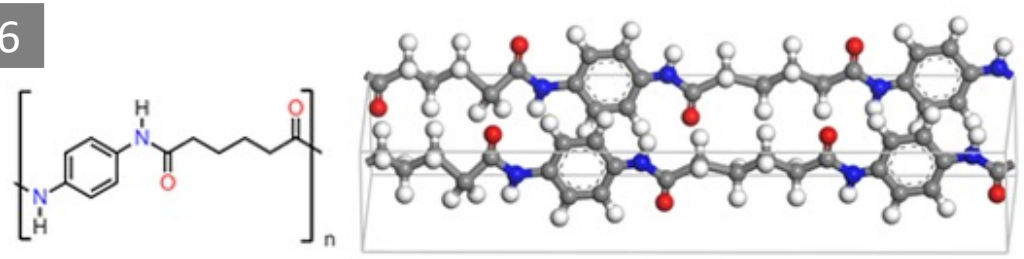
PPTA



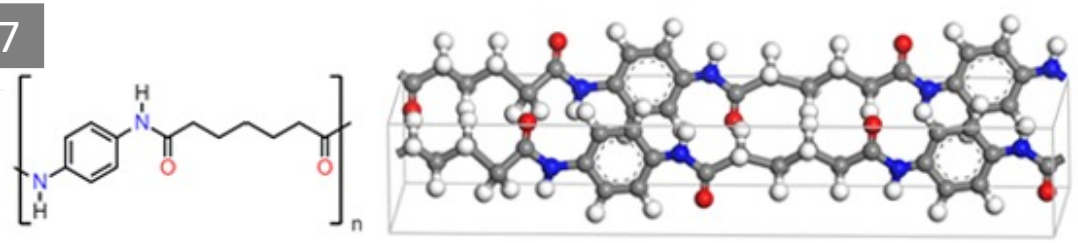
PAP5



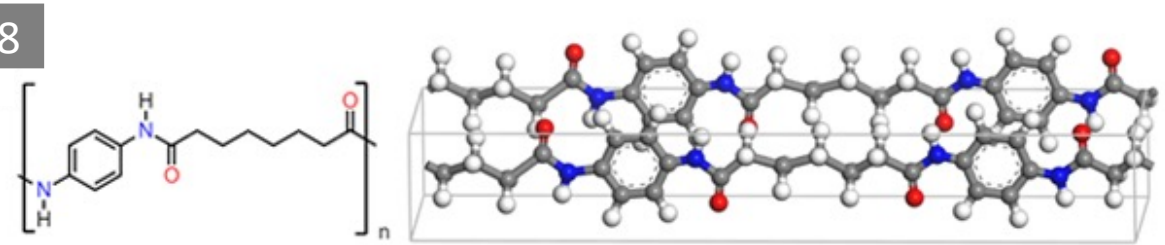
PAP6

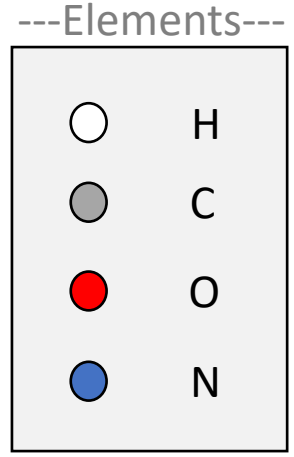


PAP7



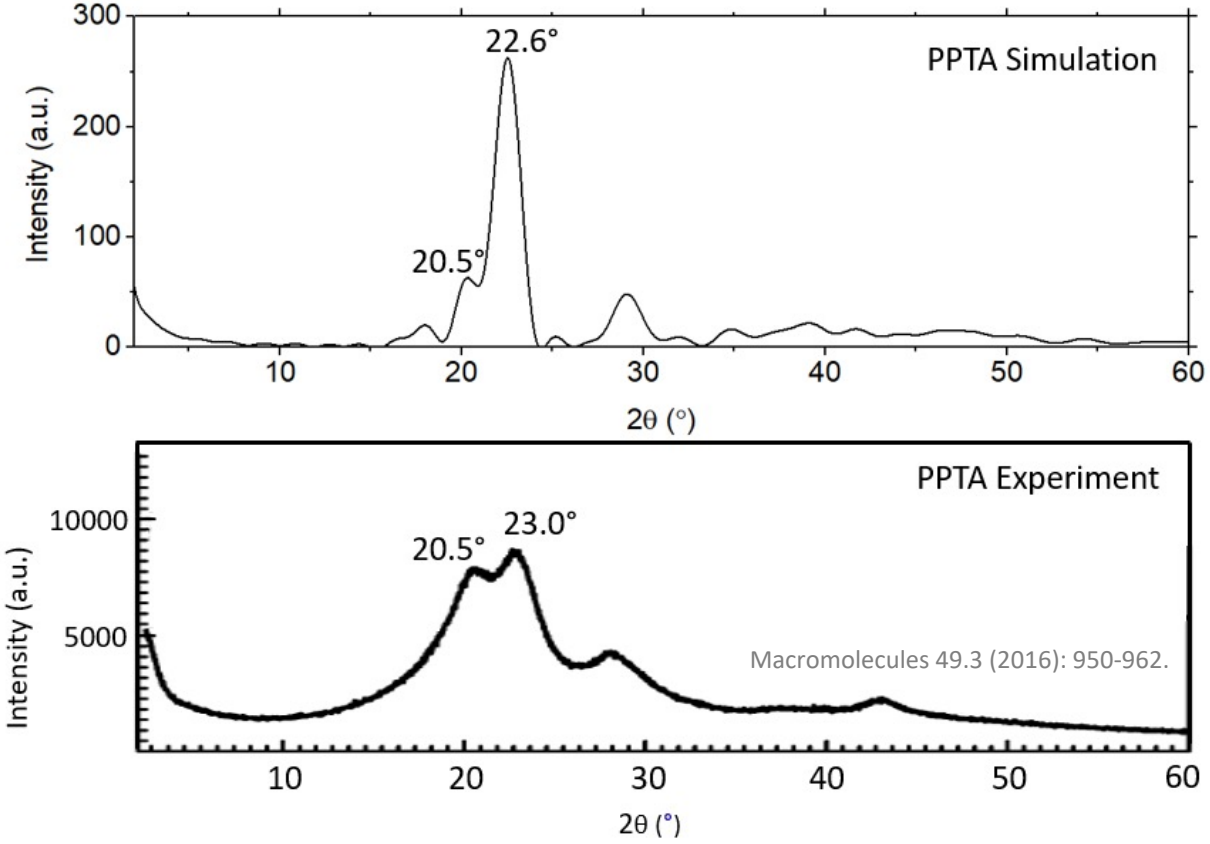
PAP8



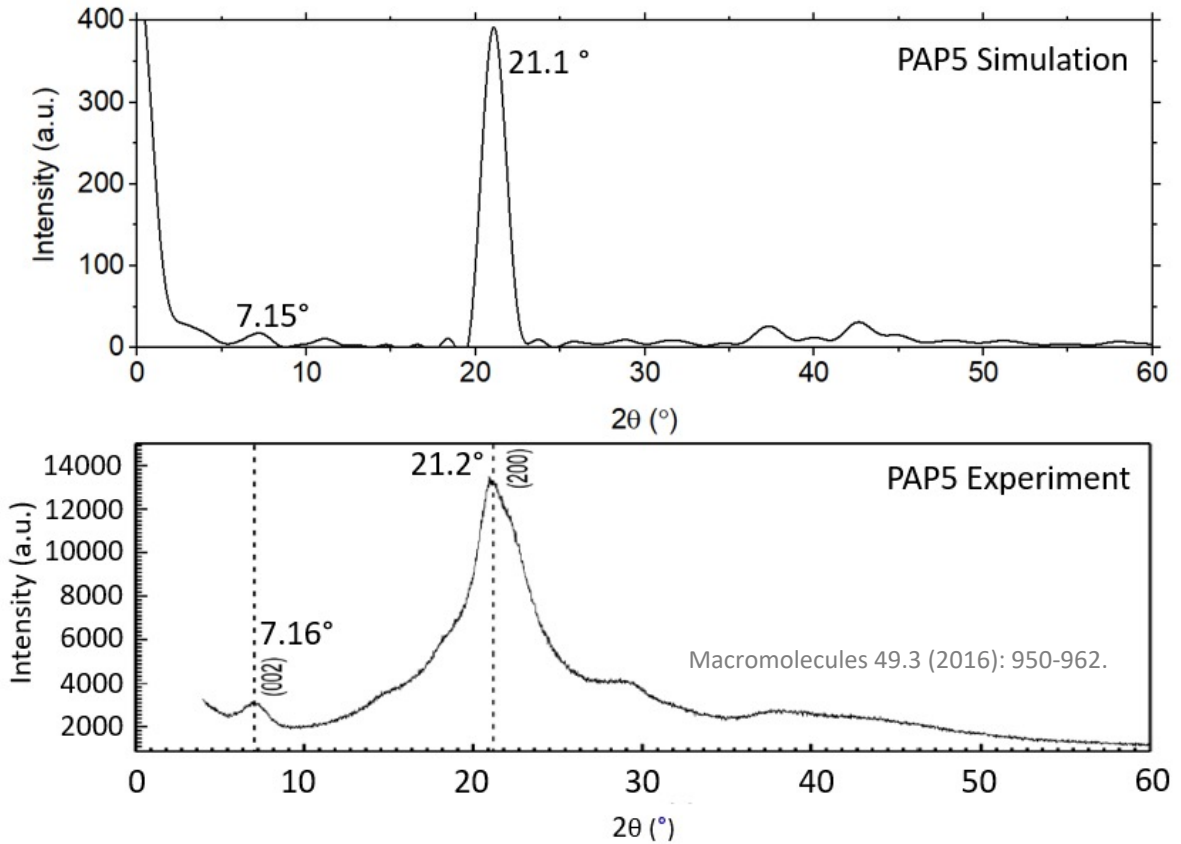


- The initial structures are manually tuned to match the experimental XRD patterns
- Note that they are not identical because the MD models are perfect crystals

PPTA

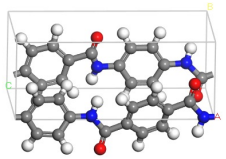


PAP5

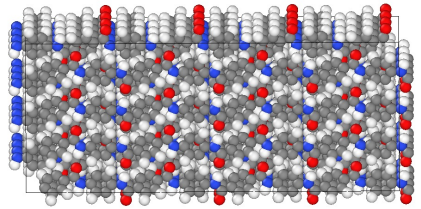


Methods >> Simulation Protocol

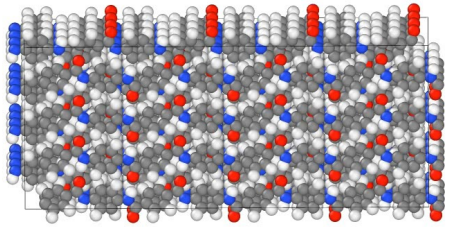
1. Create 1x1x1 unit cell model in Material Studio



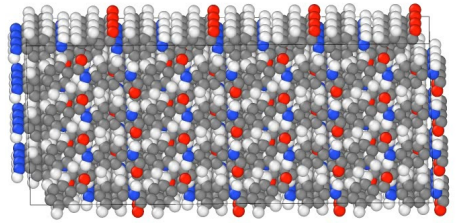
2. Replicate unit cell to 4x4x4 in LAMMPS



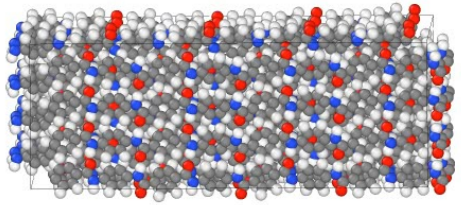
3. Energy minimization



4. Equilibration until reaching steady-state

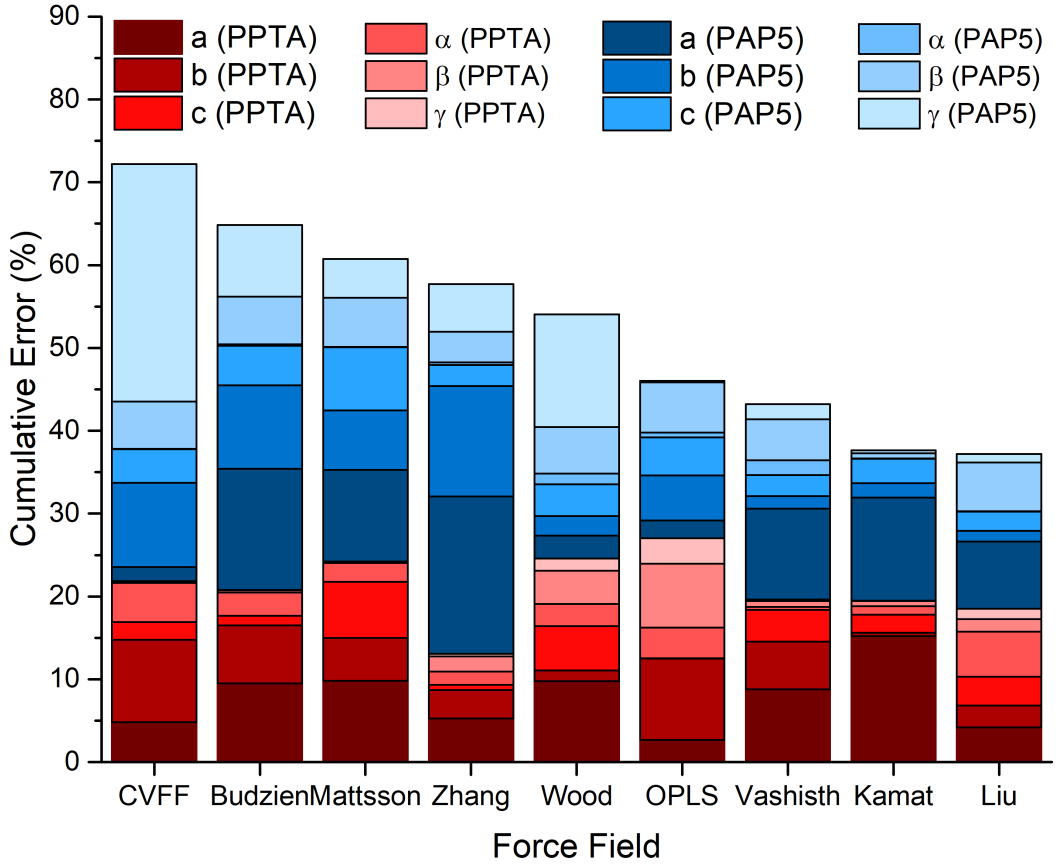


5. Stress-strain simulation



Polyamide	Unit Cell Lattice Parameters					
	a (nm)	b (nm)	c (nm)	α (˚)	β (˚)	γ (˚)
PPTA	0.787	0.518	1.29	90	90	90
PAP5	0.850	0.470	2.48	90	85	90

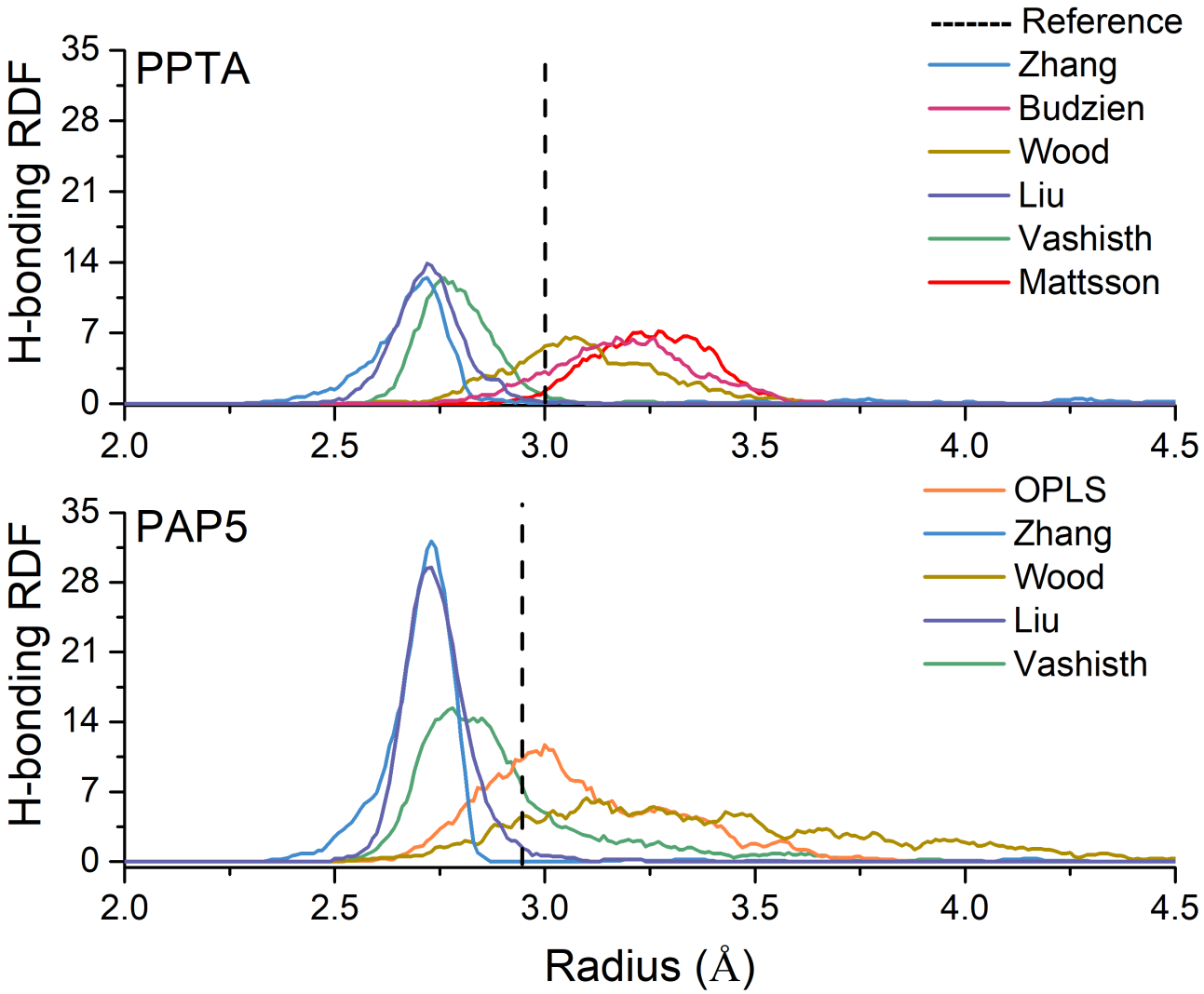
Macromolecules 49 (2016): 950-962.



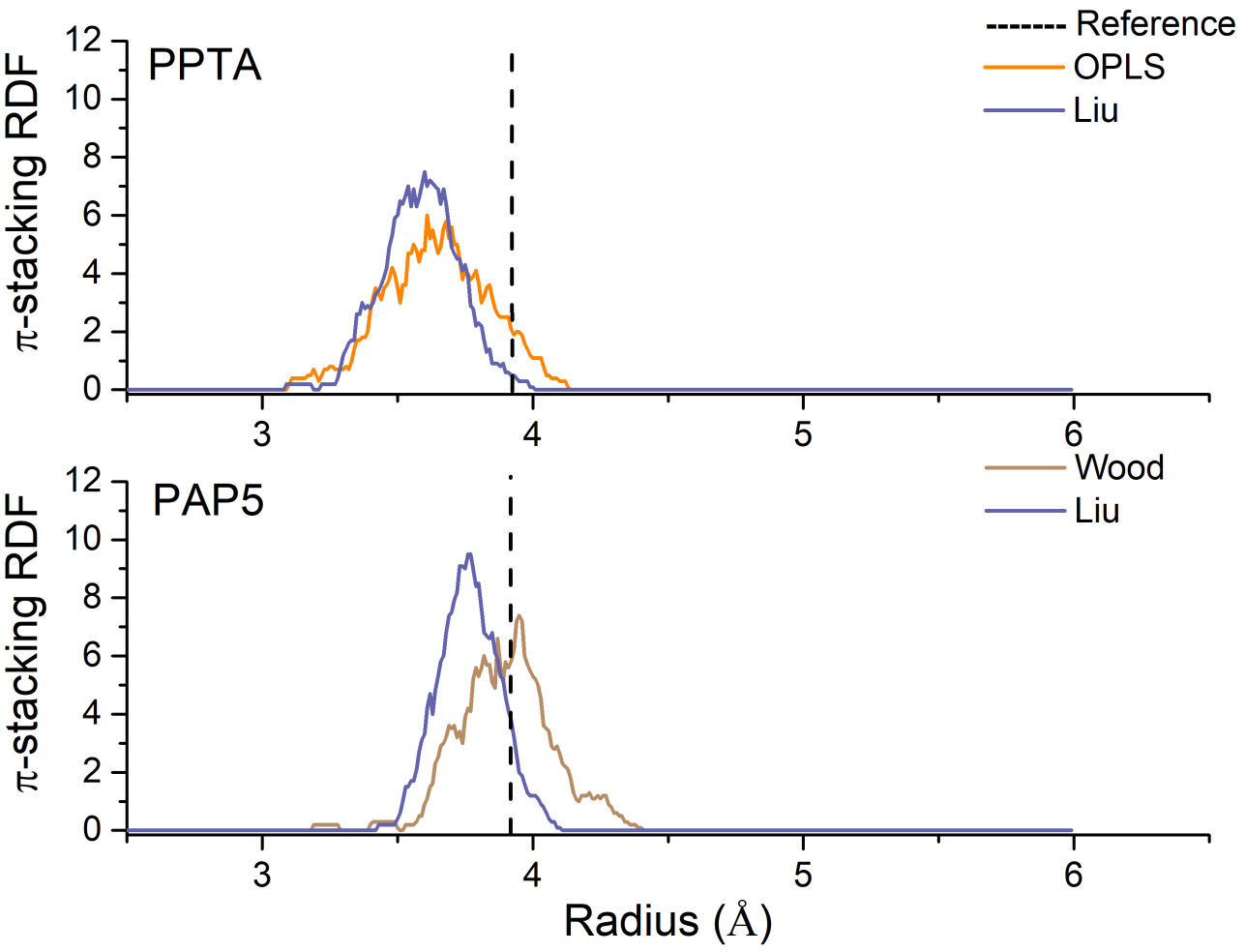
- Comparison of the accuracy (error) and stability (deviation) of **7** reactive potentials and **2** non-reactive potentials.
- CVFF has the largest error and especially large error in γ of PAP5

Reactive ReaxFF Potentials:

Mattsson et al. Phys. Rev. B 2010, 81, 054103.
Zhang et al. J. Phys. Chem. B 2009, 113, 31, 10770-10778.
Kamat et al. J. Phys. Chem. A 2010, 114, 48, 12561-12572.
Wood et al. J. Phys. Chem. A 2014, 118, 5, 885-895.
Vashisth et al. *J. Phys. Chem. A* 2018, 122, 32, 6633-6642.
Liu et al. *J. Phys. Chem. A* 2011, 115, 11016-11022.
Budzien et al. *J. Phys. Chem. B* 2009, 113, 13142-13151.



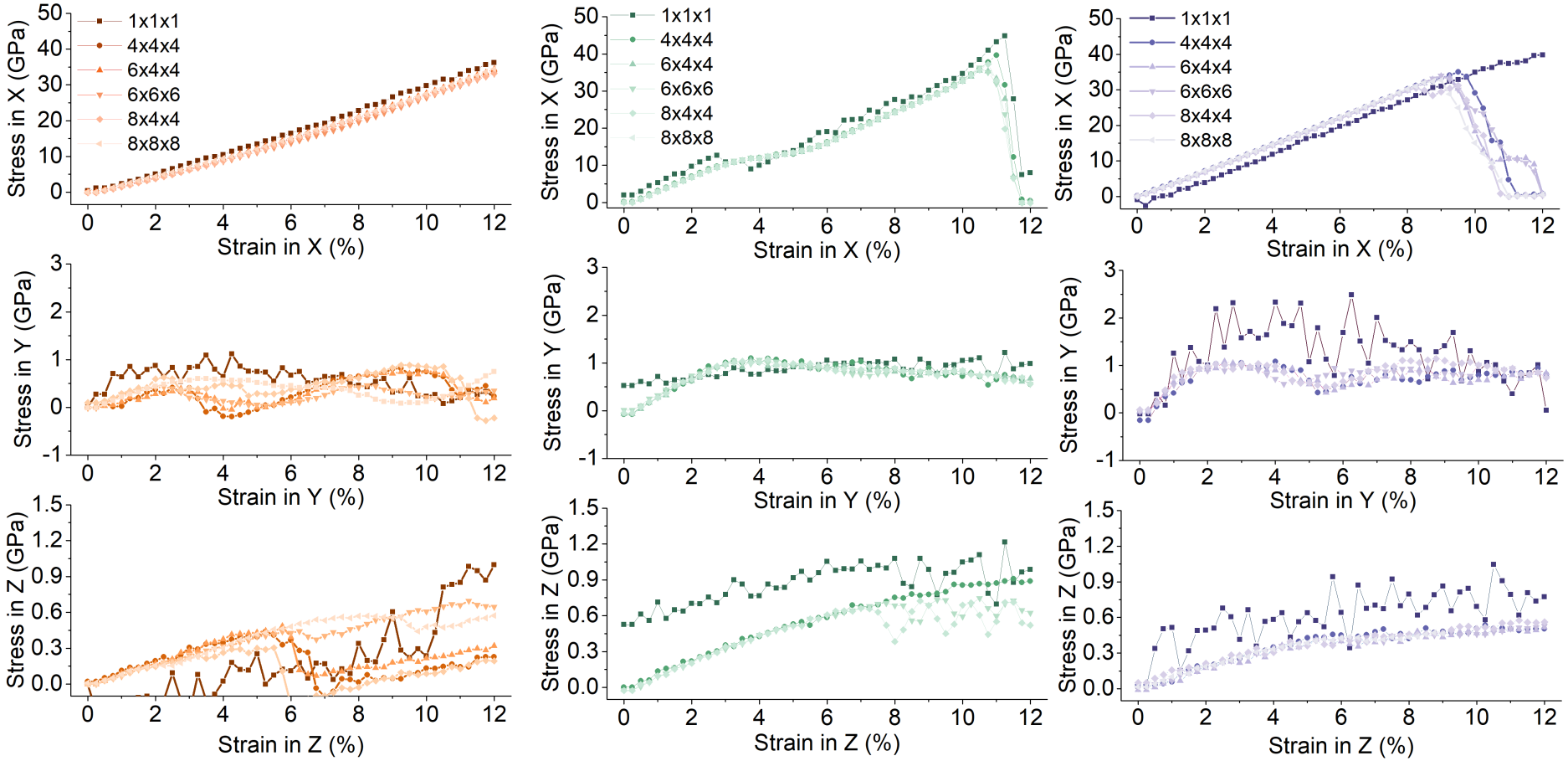
- Comparison of O-N radial distribution functions calculated for PPTA and PAP5
- Close-to-reference, tall, and narrow peaks are desirable
- For PPTA, the best potentials are Wood, Budzien, Mattsson, Zhang, Vashisth, and Liu
- For PAP5, the best are OPLS, Wood, Zhang, Vashisth, and Liu

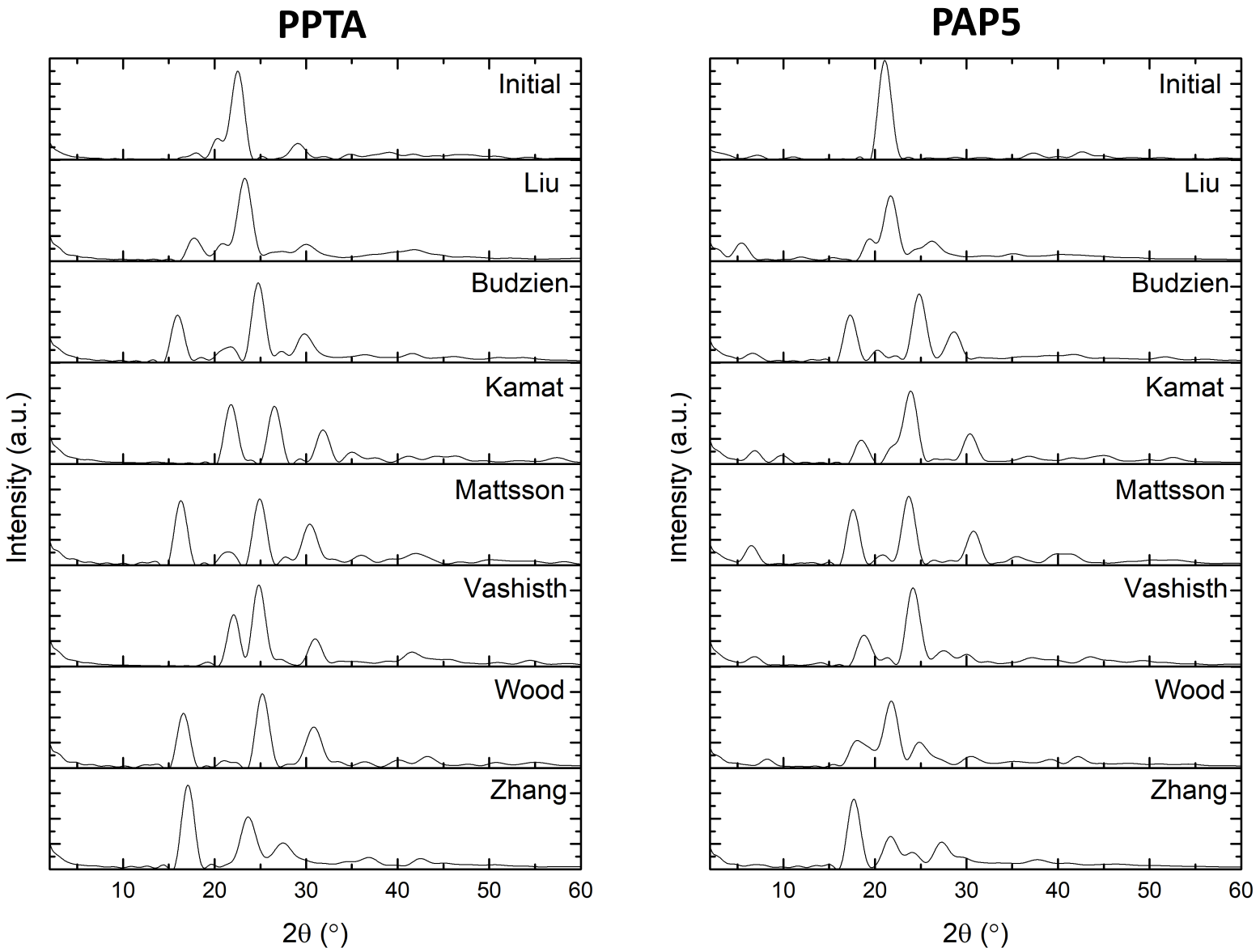


- Comparison of O-N radial distribution functions calculated for PPTA and PAP5
- Close-to-reference, tall, and narrow peaks are desirable
- For PPTA, the RDF peaks of Liu and OPLS are the closest to the reference value
- For PAP5,Wood and Liu are the most accurate, with relatively narrow peaks

- Identify the smallest model that can be used (to maximize computational efficiency) without simulation artifact
- OPLS doesn't break at all
- Vashisth shows fluctuations between 7-12% strain
- Size 4x4x4 and the ReaxFF Liu potential are suitable for the stress-strain response of PPTA and PAP5

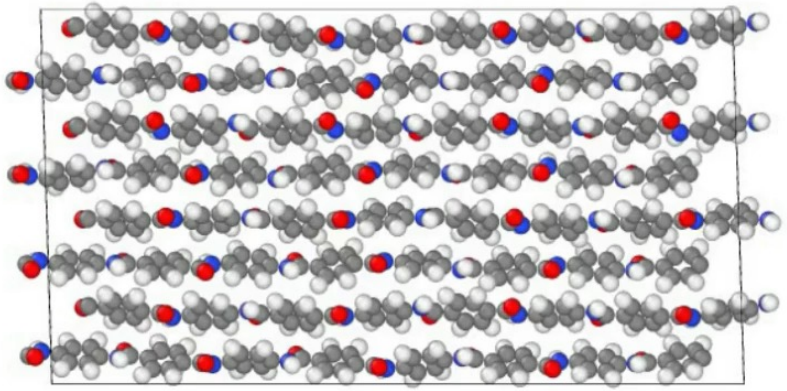
Non-reactive OPLS | **ReaxFF Vashisth** | **ReaxFF Liu**



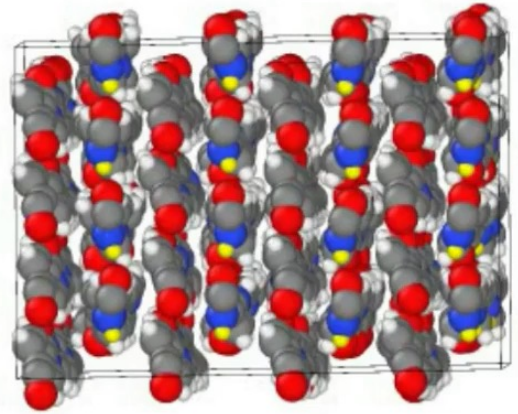


- Comparing the XRD patterns of after equilibration using different force fields with the XRD patterns from the initial structures of PPTA and PAP5
- Obviously, Liu has the retains the initial structures better for both PPTA and PAP5, i.e., reproduce the experimental structures of PPTA and PAP5 better than the other force fields

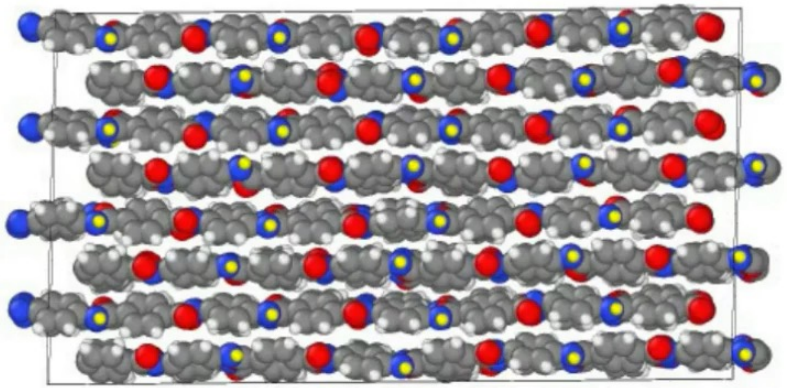
PPTA



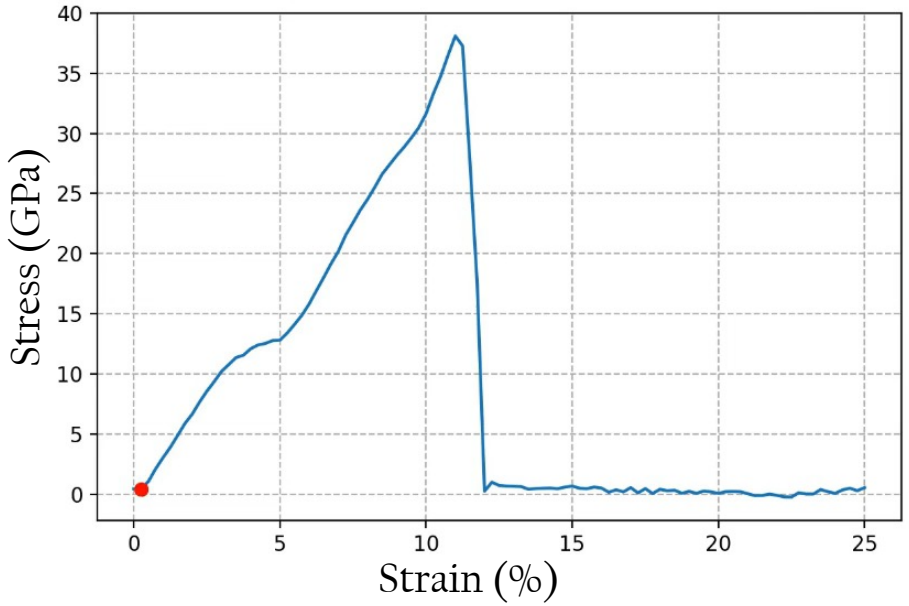
Top View



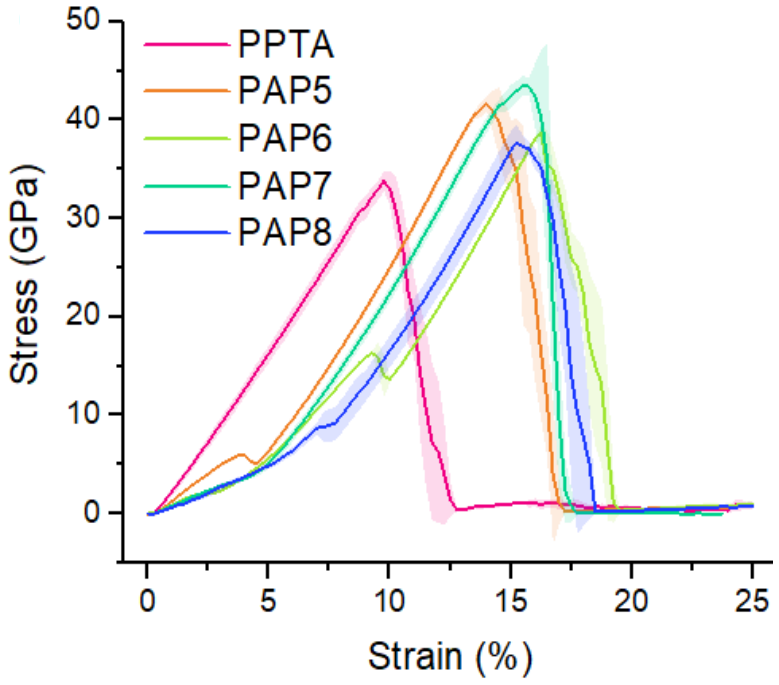
Side View

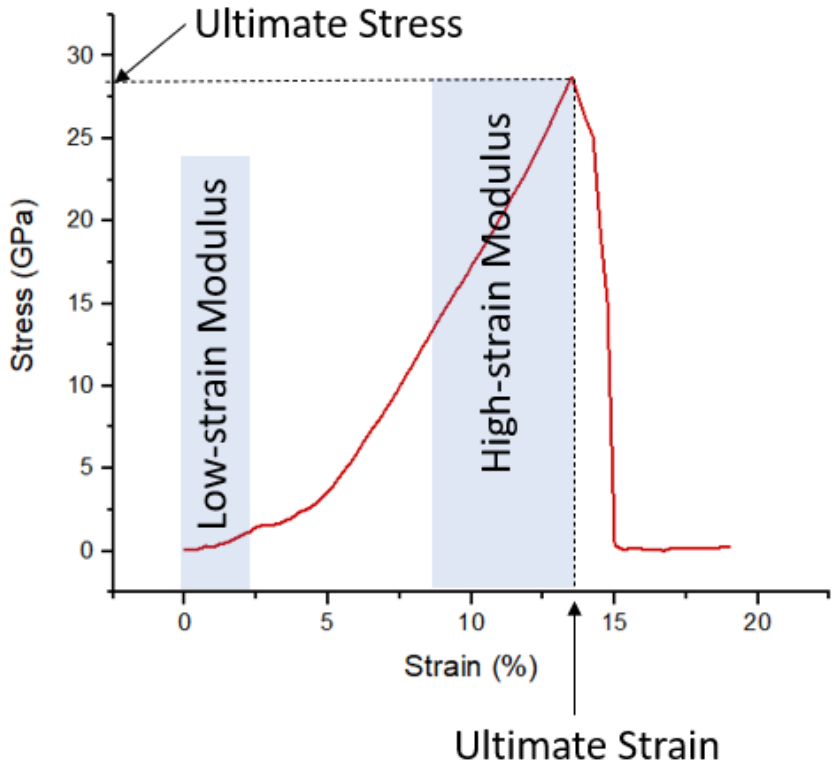


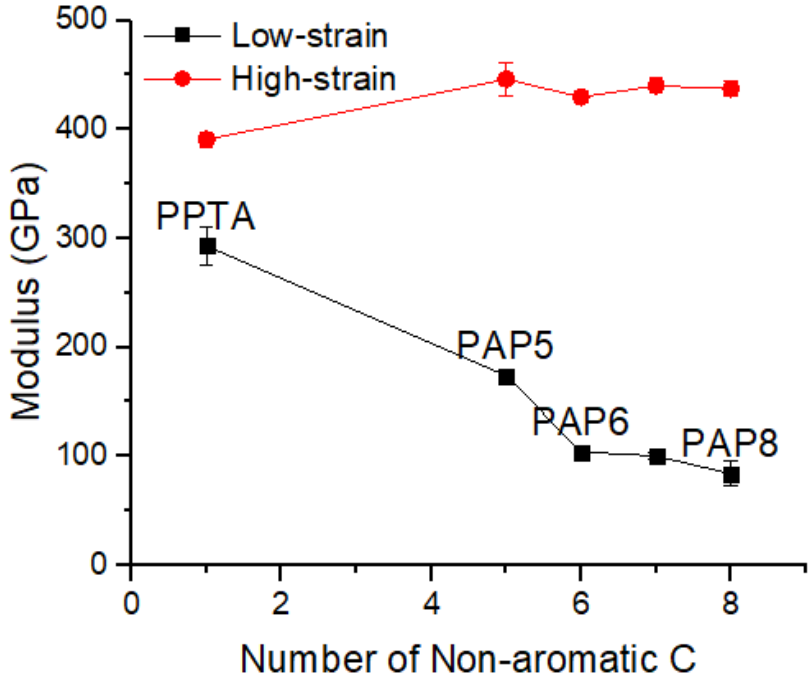
Front View



- With the selected ReaxFF Liu potential, we performed stress-strain simulations for PPTA and 4 PPTA-related aromatic-aliphatic polyamides (PAP5 and PAP6 are from the Deshmukh paper [1])
- Low-strain modulus lower than high-strain modulus
- Low-strain modulus decreases with increasing number of non-aromatic C atoms
- High-strain modulus is essentially independent of the number of non-aromatic C atoms





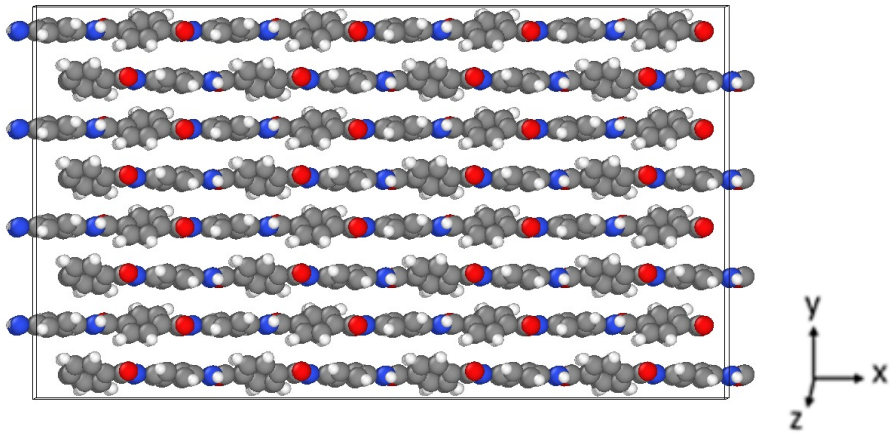


[1] *Macromolecules* 49.3 (2016): 950-962.

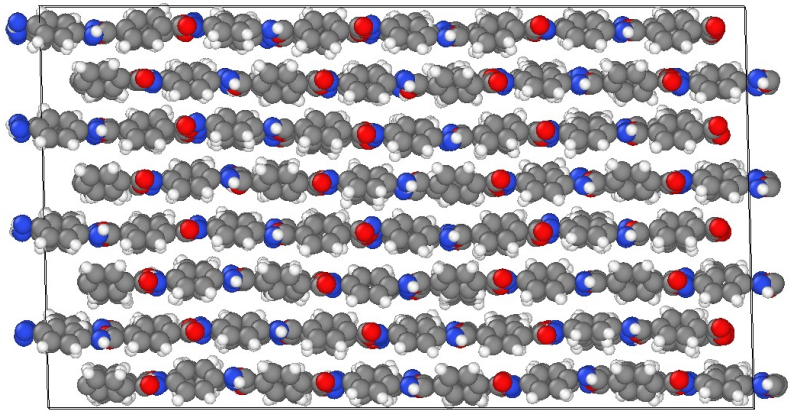
- After equilibration, the chains become wavy, especially for polymers with more non-aromatic C

PPTA

Initial Structure

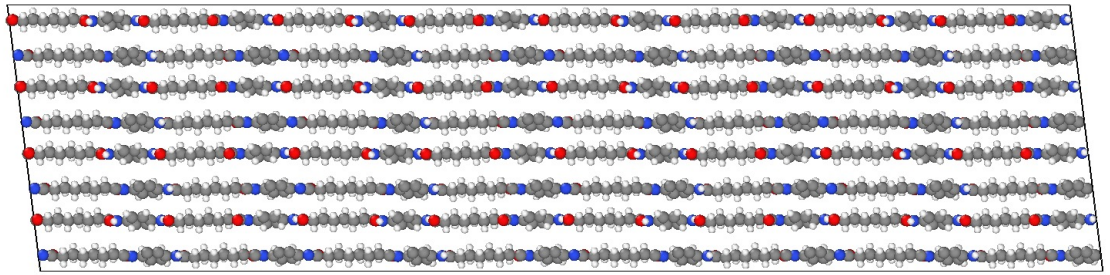


After Equilibration

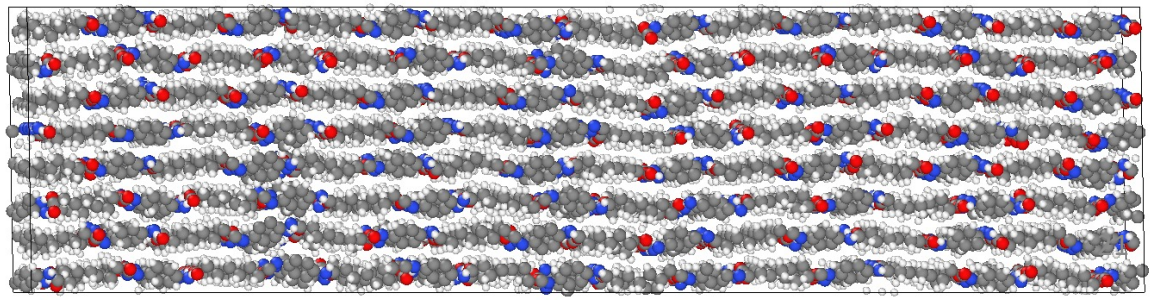


PAP8

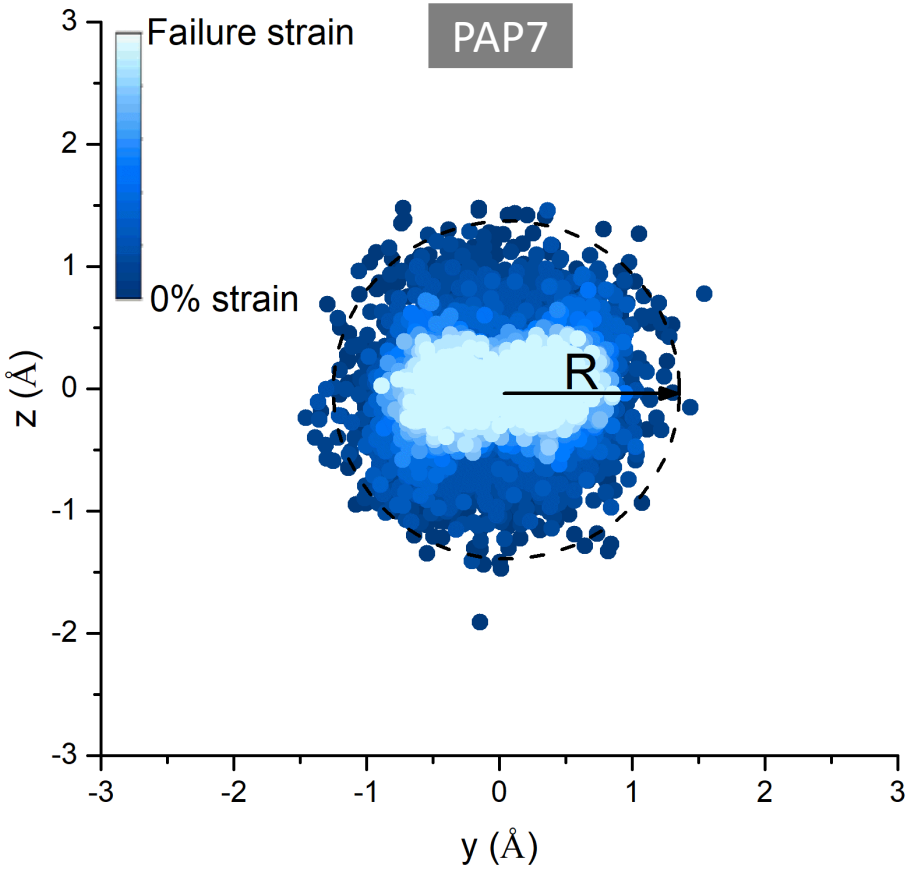
Initial Structure

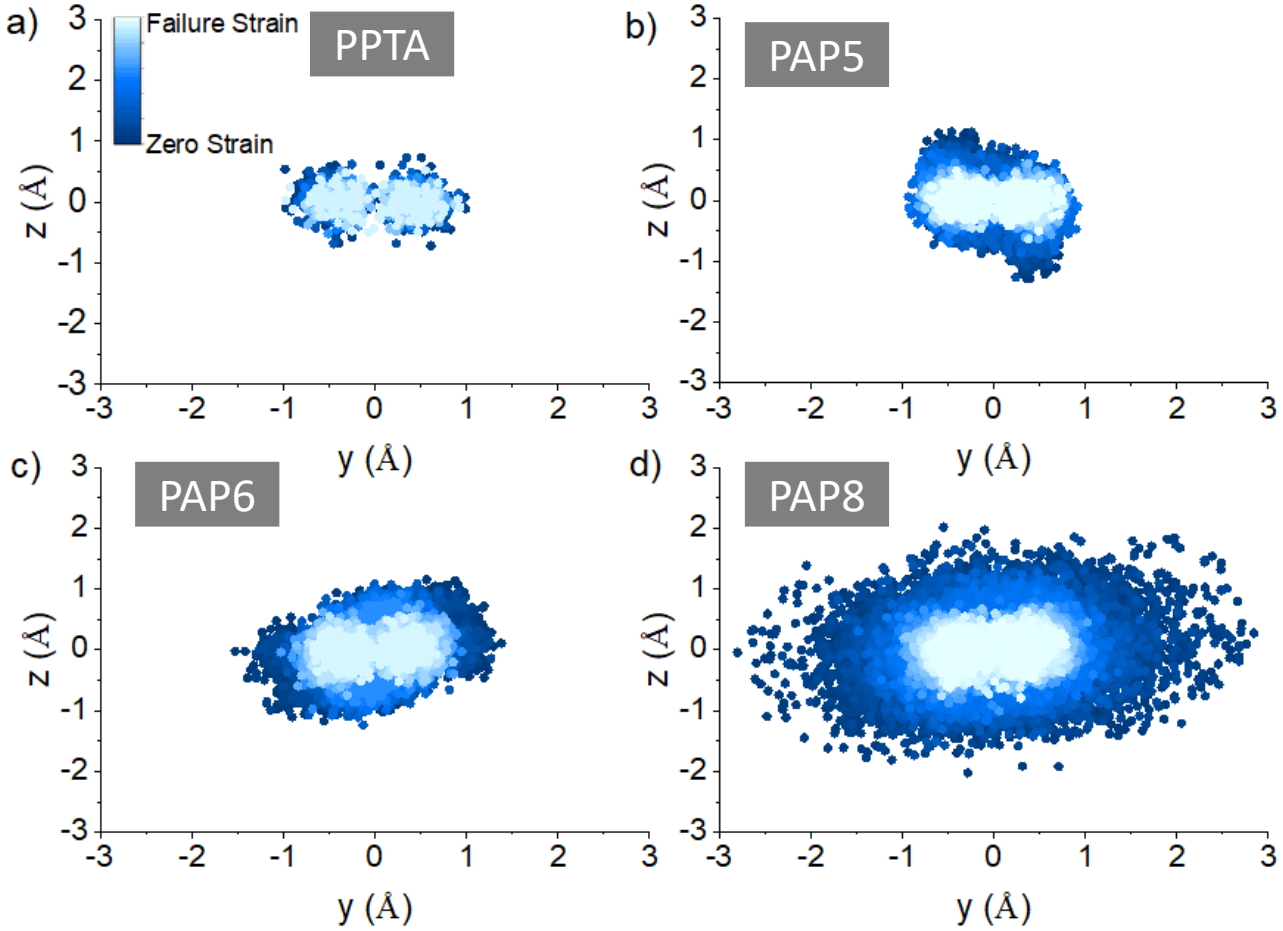


After Equilibration

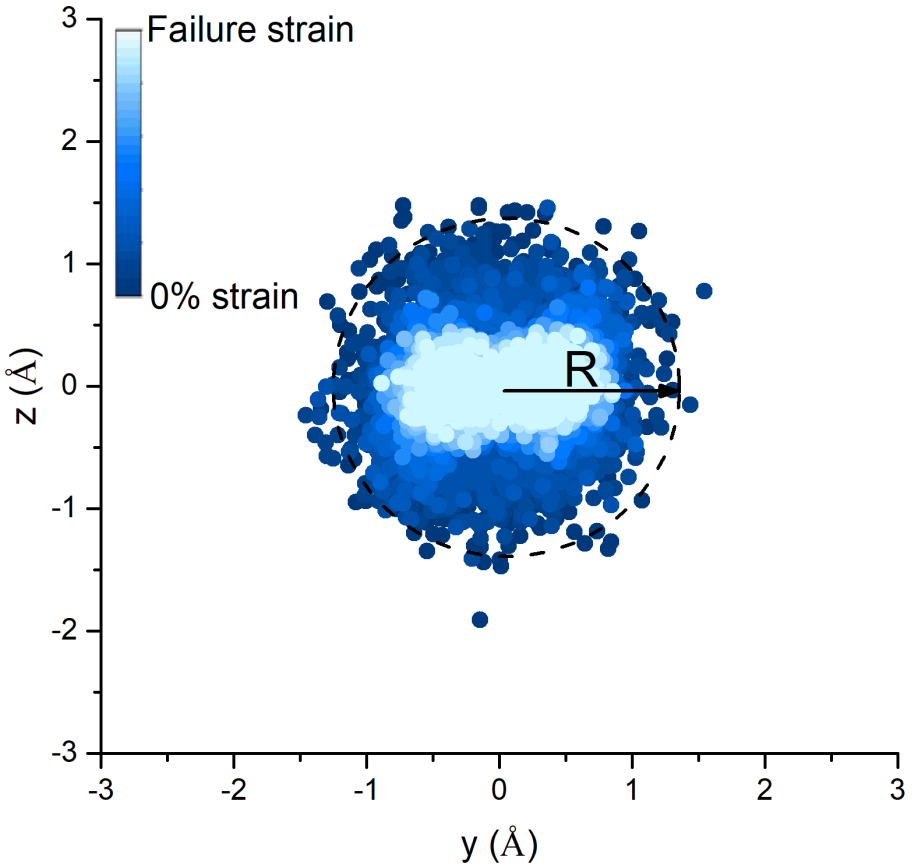


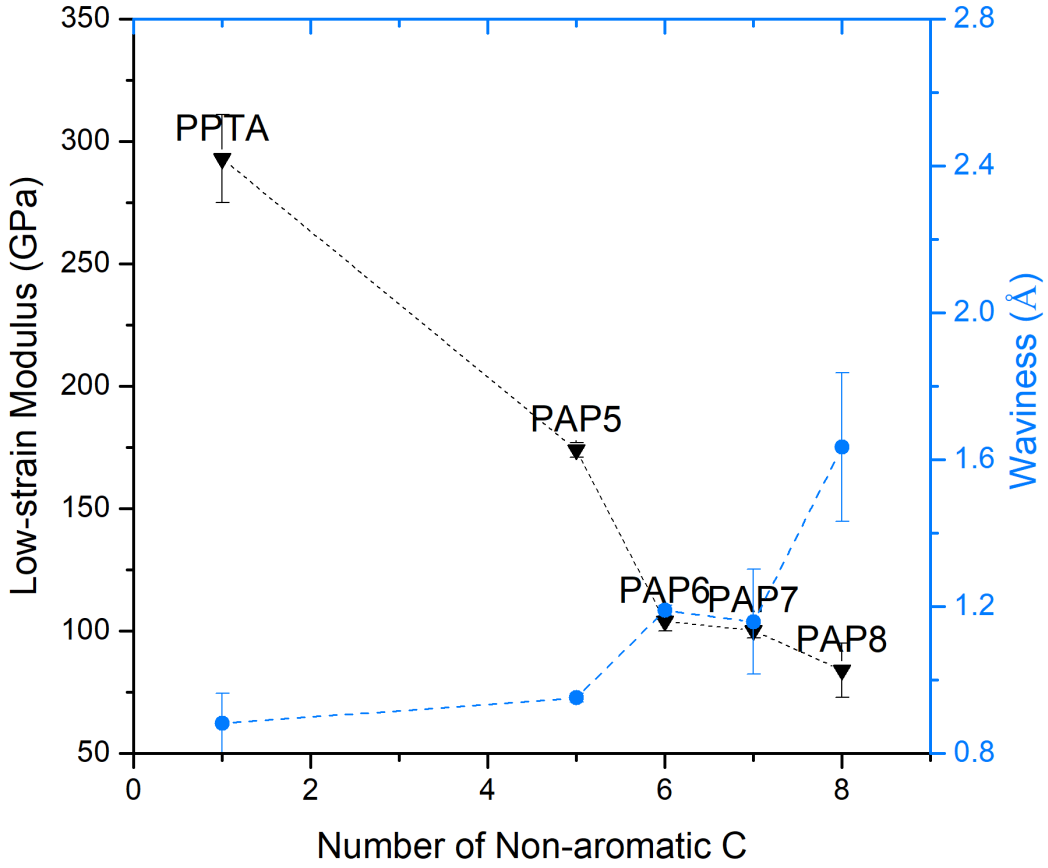
- Side view (yz-plane) of the polymers (only backbone C and N are shown)
- As the number of non-aromatic C increases, the atom cloud spreads out more (more wavy chains)





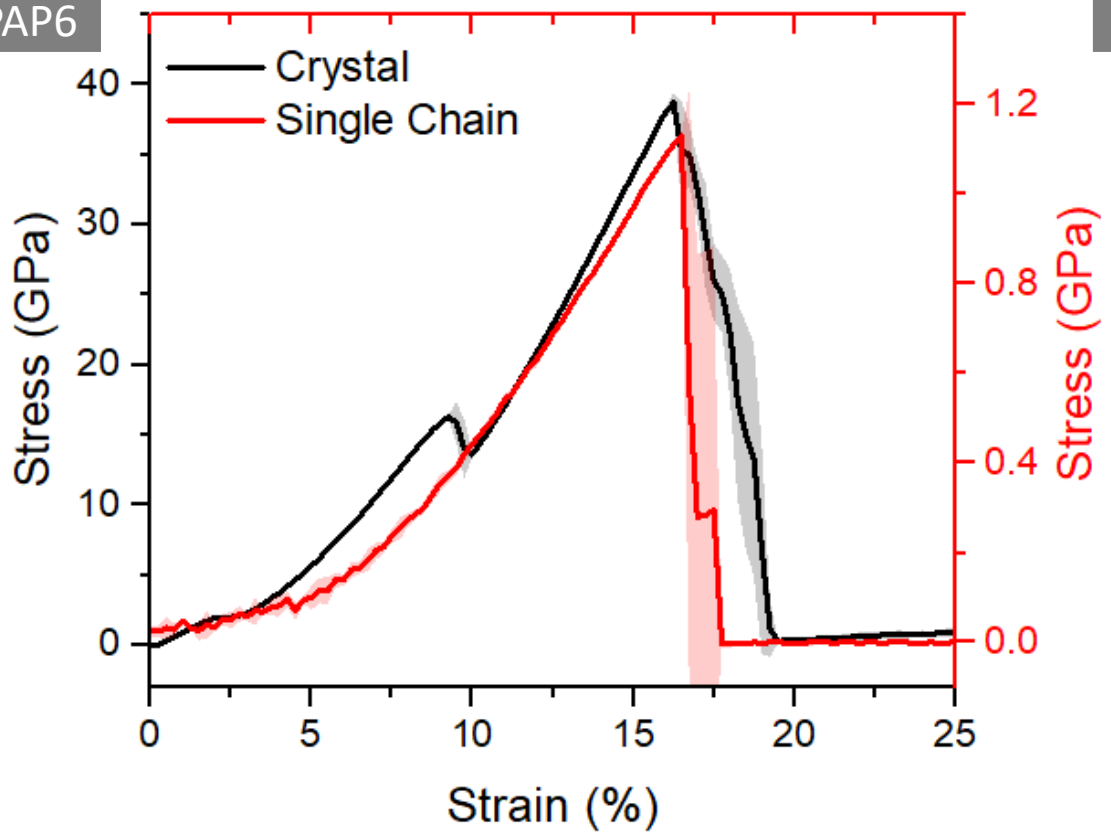
- The decrease in modulus with chain length is due to increasing waviness of the polymers
- Waviness is due to the methylene groups acting as spacers between the hydrogen-bonded amide groups, which increases the conformational freedom of the polymer chains
- More waviness decreases stiffness because force resistant to stretch has less components in the chain direction



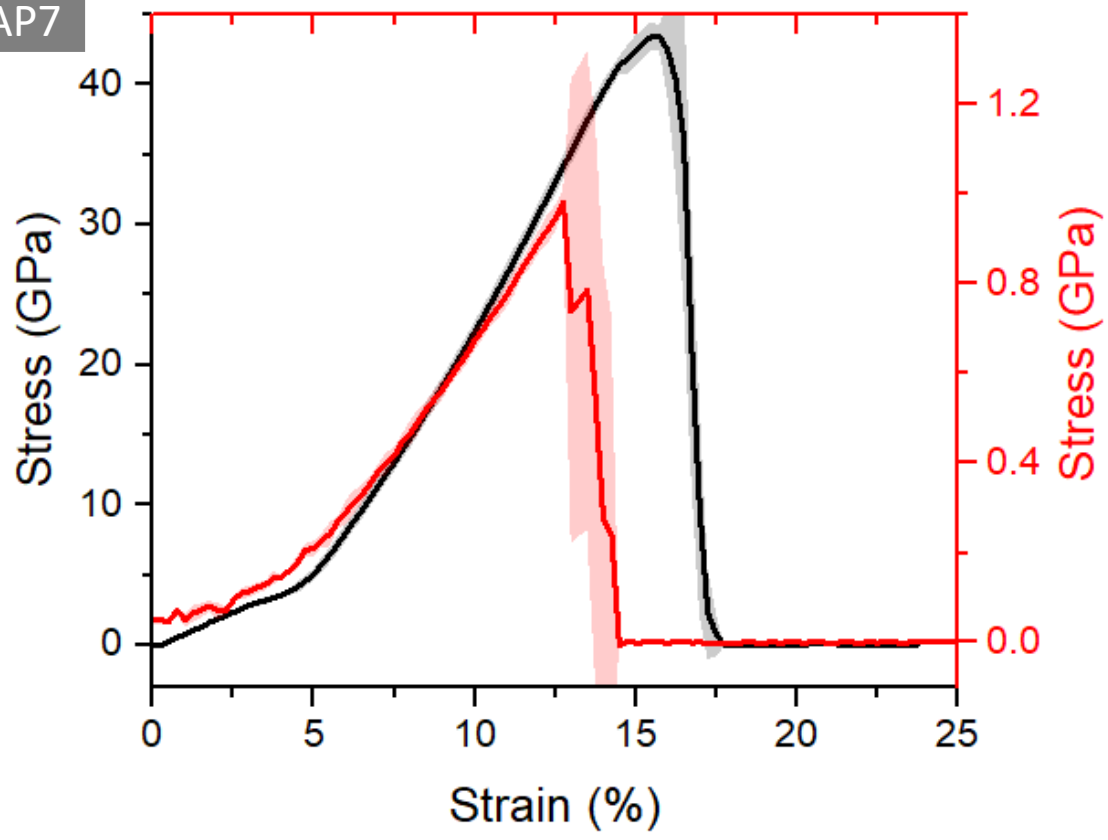


- Both single chain and crystals exhibit lower stiffness at low strain than high strain and a gradual increase in stiffness around 5% strain; this indicates the behavior is due to intrachain processes
- For the PAP6 crystal only, there is a sharp transition from low to high strain behavior observed around 10% strain
- This suggests there are odd-even effects and that they are due to interchain processes

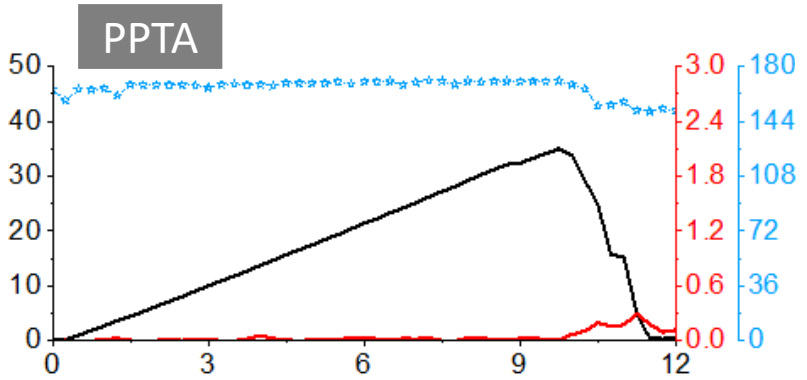
PAP6

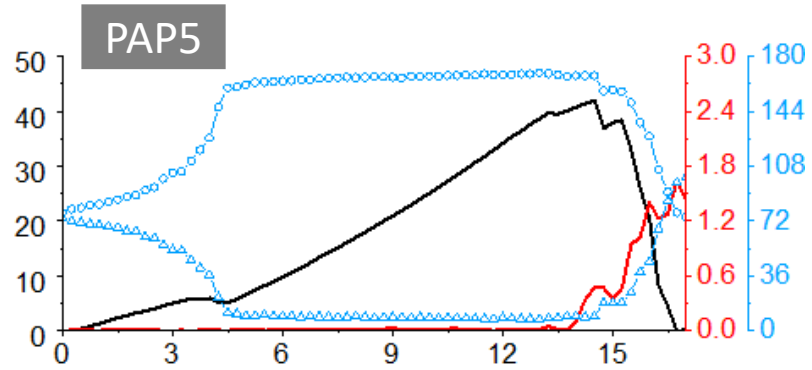


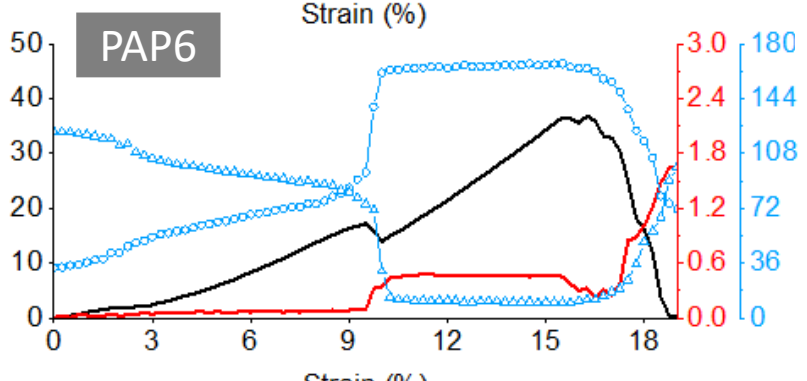
PAP7

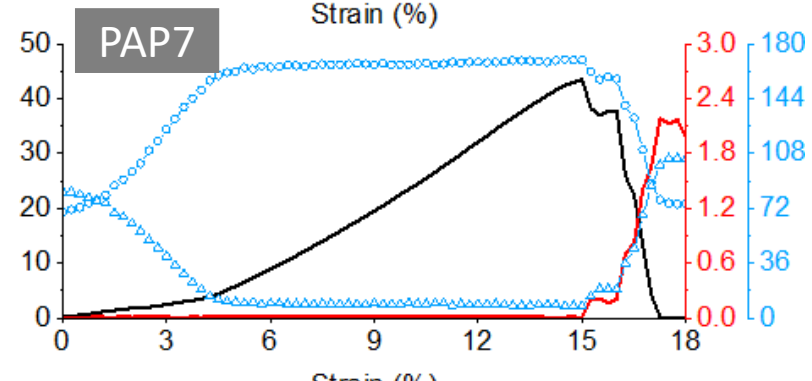


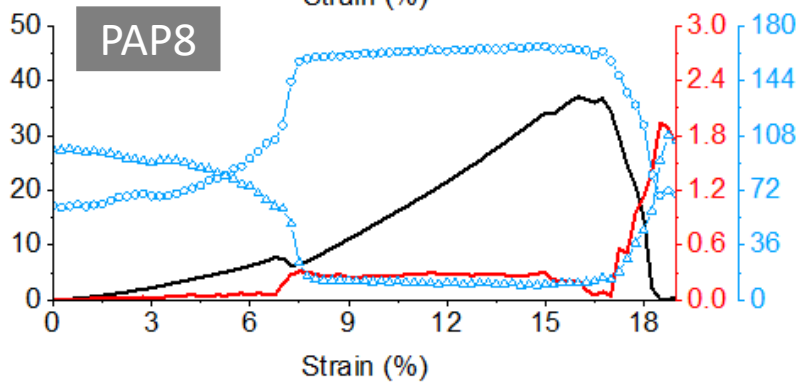
- The gradual increase in stiffness exhibited by all polymers (except PPTA) correlates well with changes in the dihedral angles, indicating the low strain is accommodated by elongation/rotation of wavy chains
- The sharp transition exhibited by PAP6 and PAP8 correlates with intra chain slip, quantified by ring-ring distance
- These even polymers slip because they have the less stable trapezoidal structure

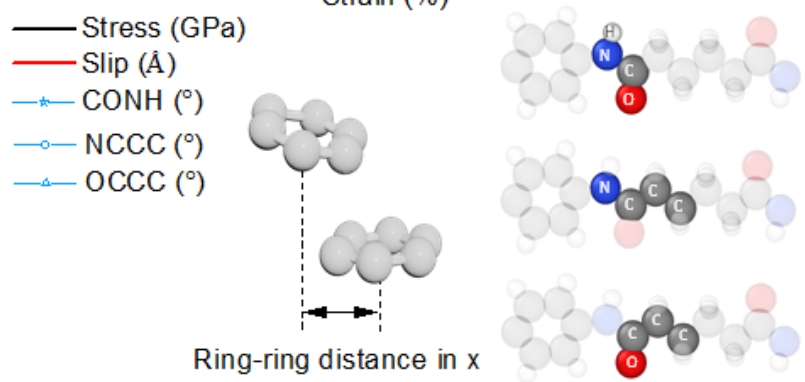






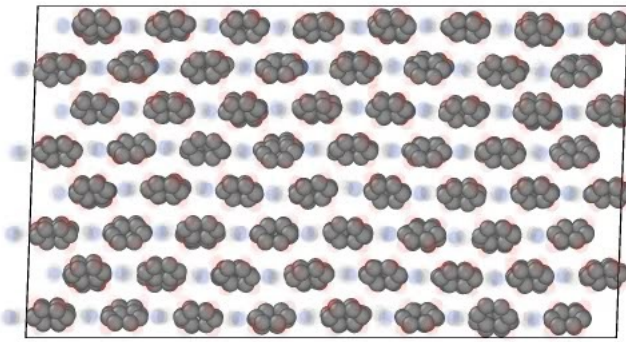




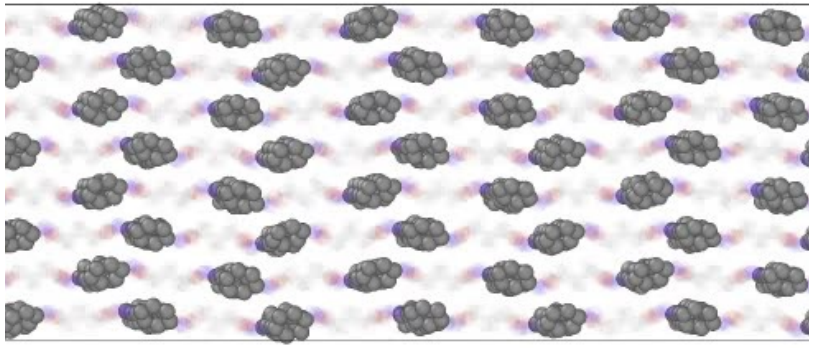


- Movies of strain simulations shown from the y-direction where all atoms except the aromatic rings are faded. Only even polymers (PAP6 and PAP8) exhibit interchain slip.

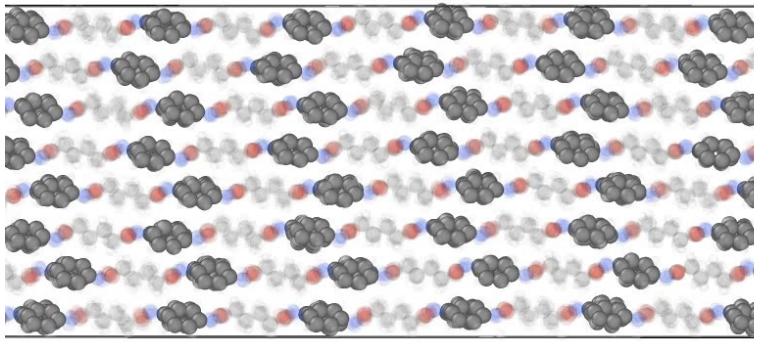
PPTA



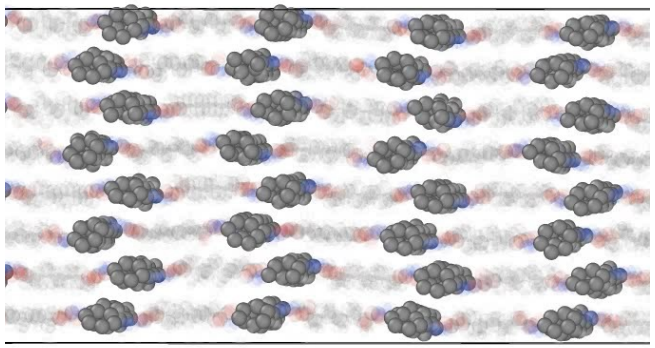
PAP5



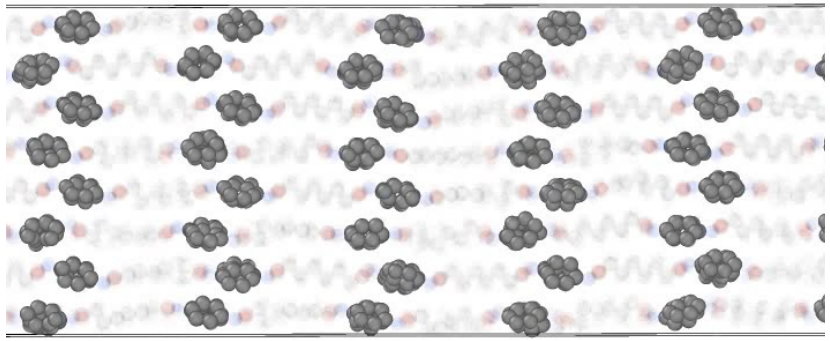
PAP6

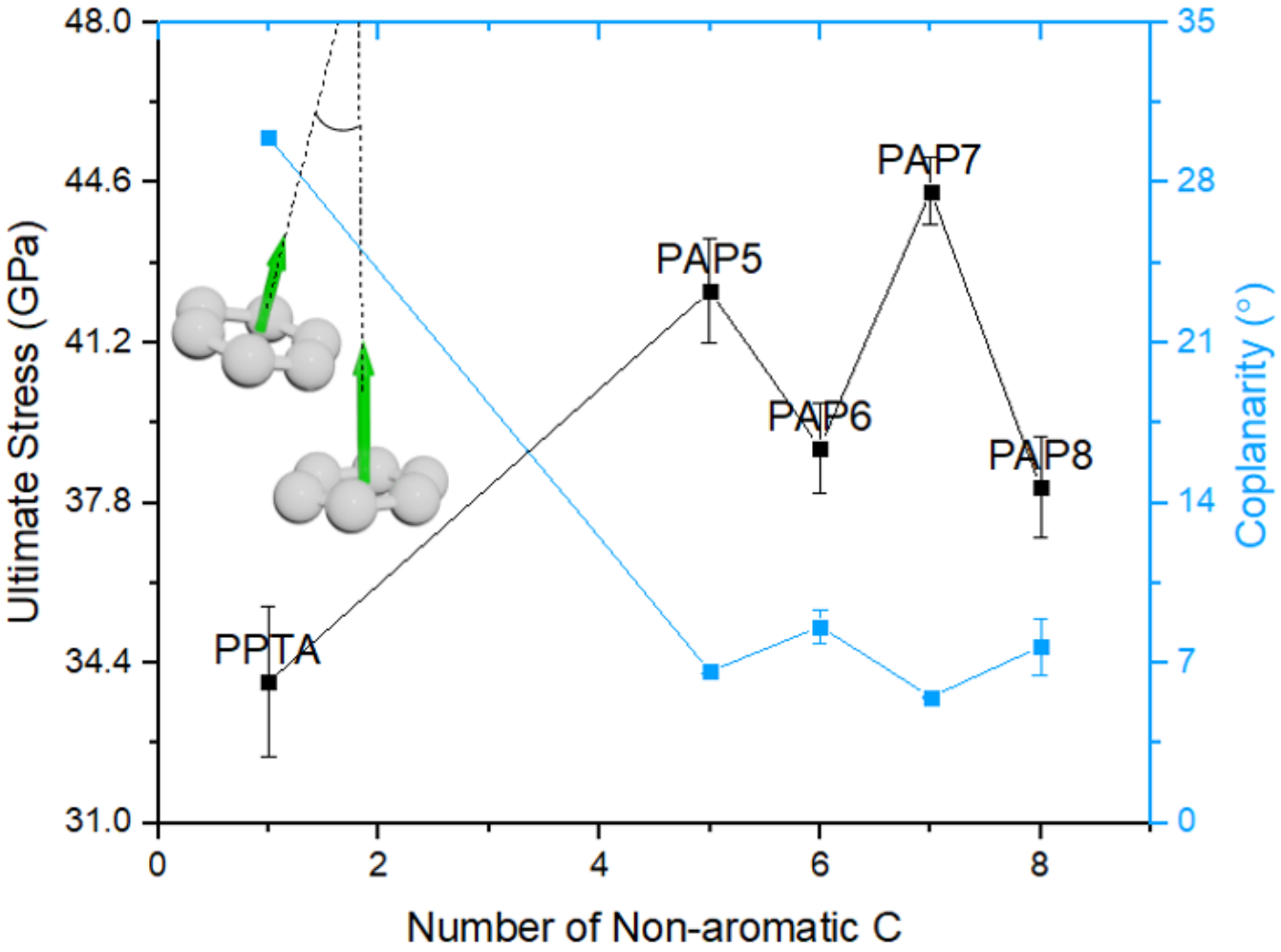


PAP7



PAP8

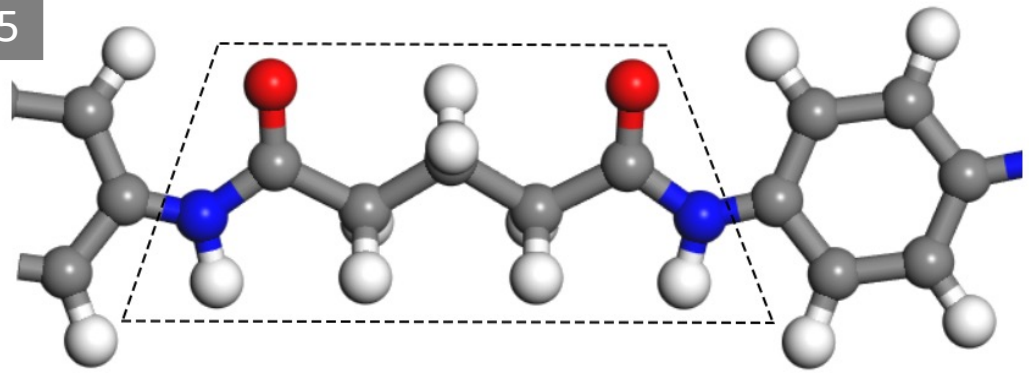




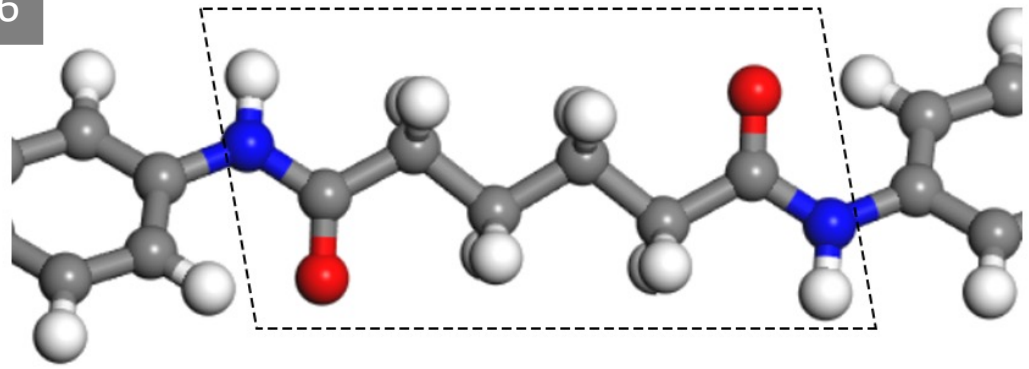
- The ultimate stress exhibits odd-even behavior where odd numbers of carbon atoms have larger strength
- Since the chains are extended at this point, and DFT results showed the bond strength is the same for all polymers, so this must be an interchain effect
- Interchain strength is determined by the coplanarity of the rings, quantified by ring-ring angle, which is lower (more aligned rings) for the polymers with odd numbers of carbon atoms, explaining their strength

- Representative snapshots of trapezoidal and parallelogrammatic structures in the backbones of odd (PAP5) and even (PAP6) polymers.
- It is an important origin of odd-even effect

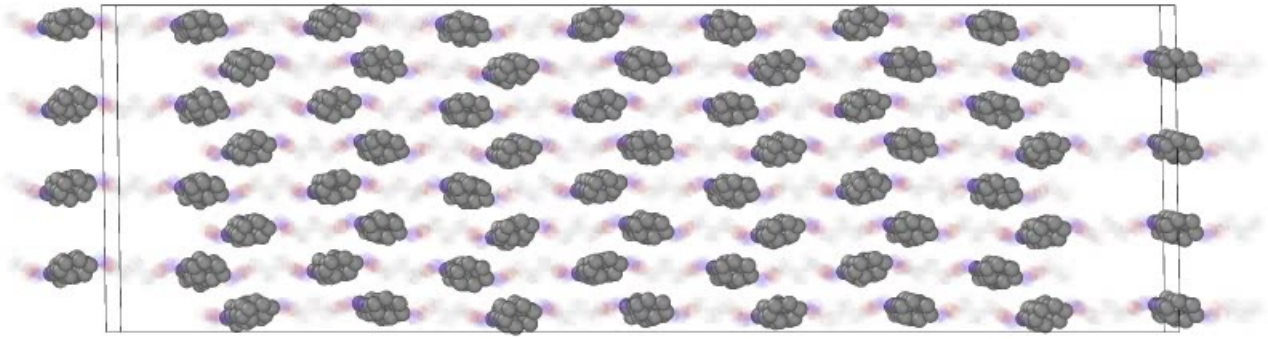
PAP5

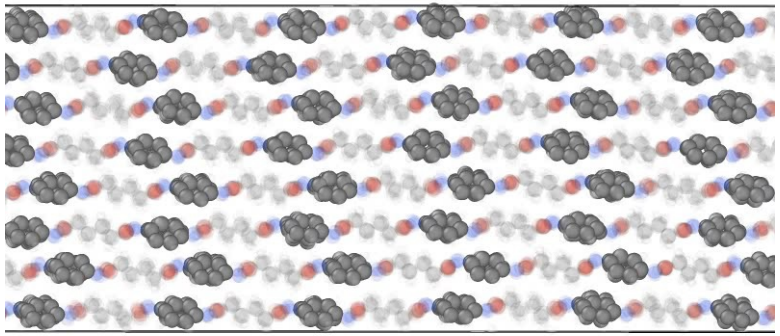


PAP6



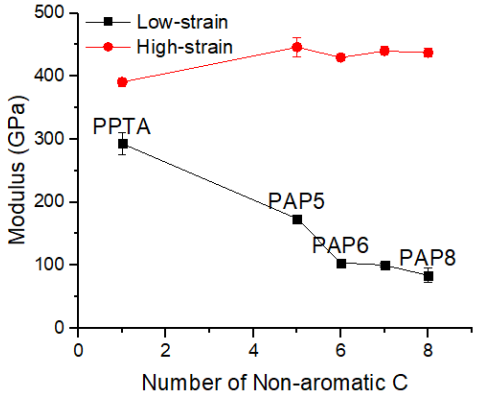
Movies of chain slip



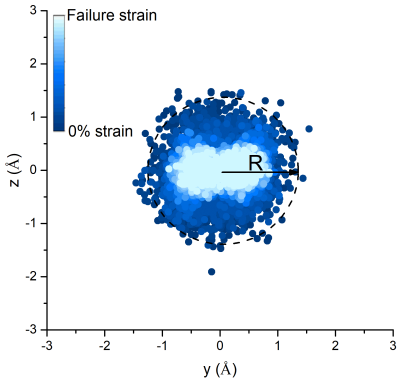


Summary of Polyamides MD Simulations

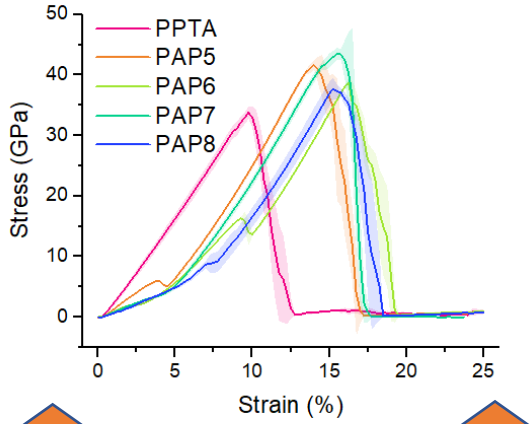
Modulus



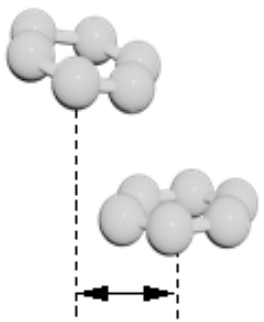
Waviness



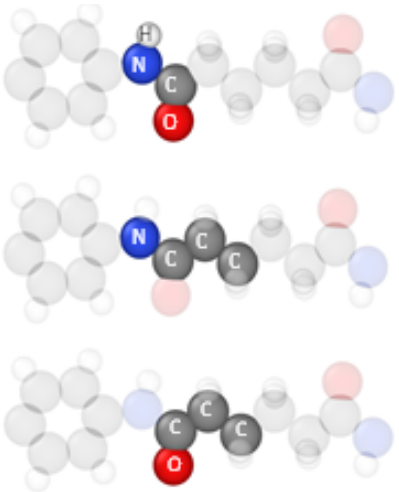
Transition



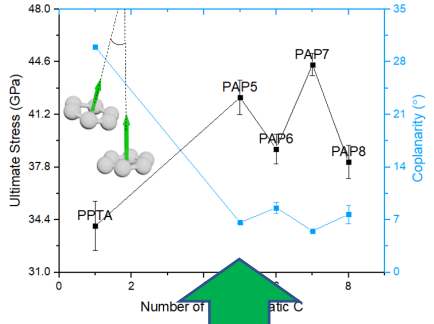
Slip



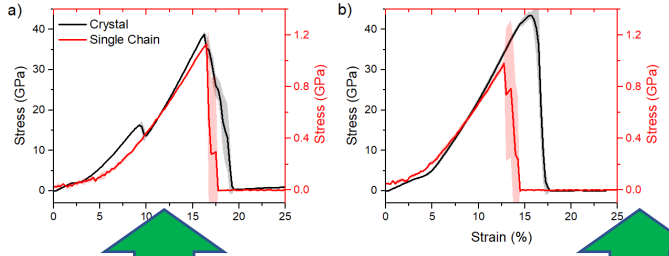
Rotation



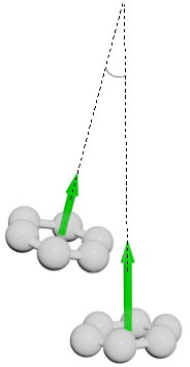
Ultimate Stress



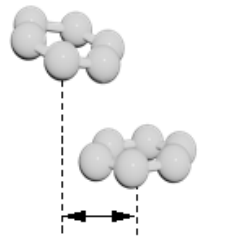
Intermolecular interactions



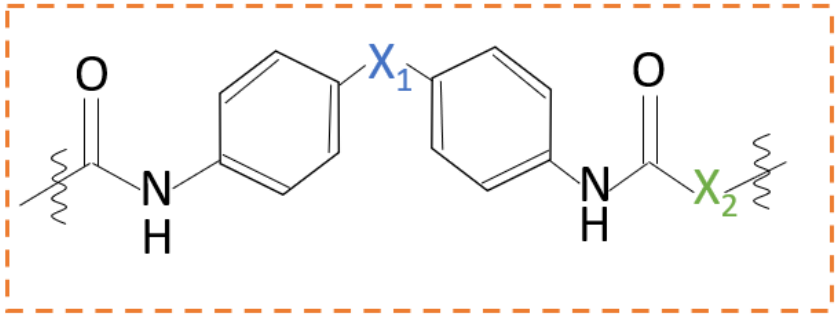
Ring-ring coplanarity



Slip



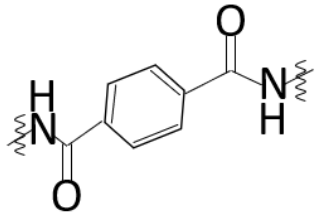
Suggestions for Future Work



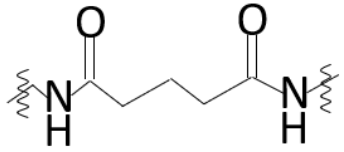
- PPTA and PAP5-PAP8 can be written in the same formula with different X_1 and X_2 groups
- X_1 and X_2 groups for PPTA and PAP5-PAP8 are shown in the following lists
- It means that the functional groups X_1 and X_2 groups affect mechanical properties

X_1:

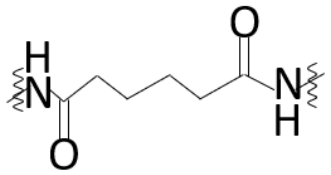
PPTA



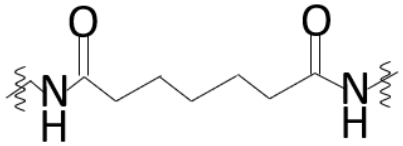
PAP5



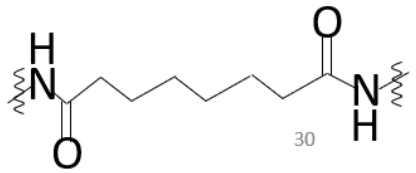
PAP6



PAP7



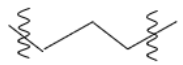
PAP8



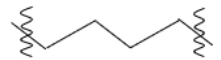
X_2:

PPTA

PAP5



PAP6



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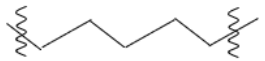

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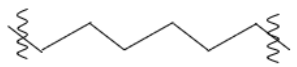
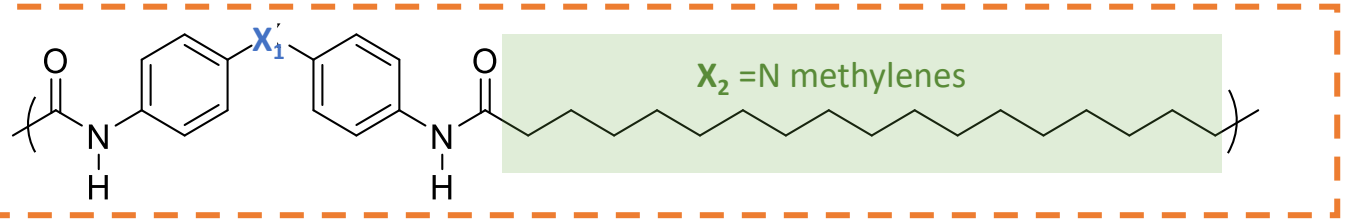


30

Suggestions for Future Work

➢ Effect of Functional Groups on Stress-strain Response



Functional Groups X_1:

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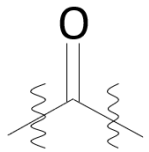
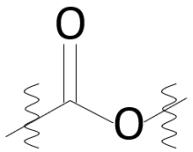
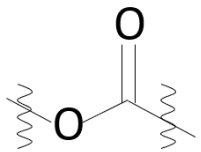
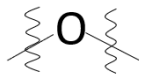
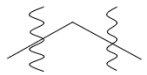
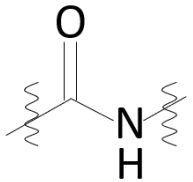
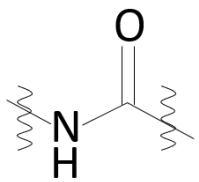
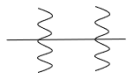
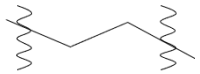
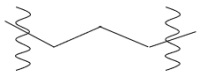
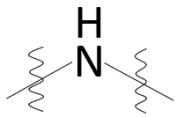
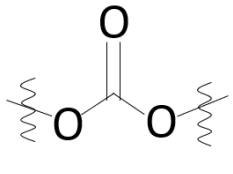
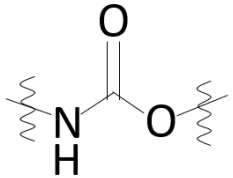
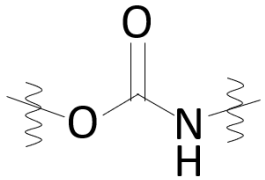
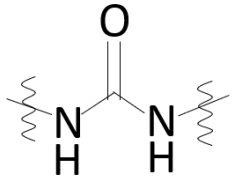
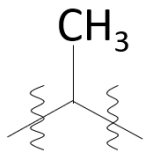
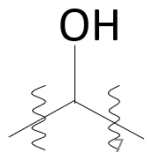
					
hPAP-idx1	**hPAP-idx1-f**	**hPAP-biphenyl**	**hPAP-Et**	**hPAP-Pr**	**hPAP-NH**
					
hPAP-carbonate	**hPAP-urethane**	**hPAP-urethane-f**	**hPAP-urea**	**hPAP-X6**	**hPAP-X7**
					

- Introducing more functional groups to study the effects on mechanical properties
- A list of 18 potential functional groups are listed on the left
- X_2 can be methylene groups with different lengths (e.g., 0-17 carbon atoms)
- Data volume: 18 x 18 = 324 different polyamides

Suggestions for Future Work

➢ **Using machine learning to build quantitative structure-properties relationship (QSPR)**

Polyamide Information

- Functional groups
- Chain length?
- Molecular weight?
- # of atoms?
- Bonds?

input

Machine Learning

output

Mechanical Properties

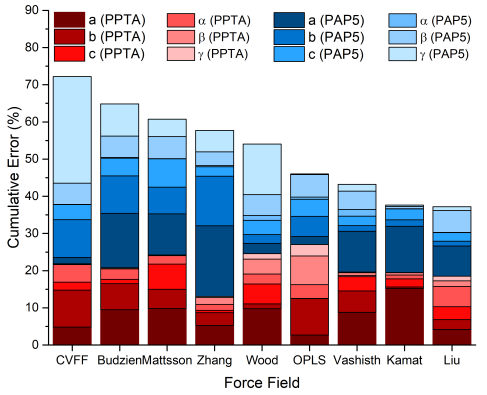
- Low-strain modulus
- High-strain modulus
- Ultimate strain
- Ultimate stress

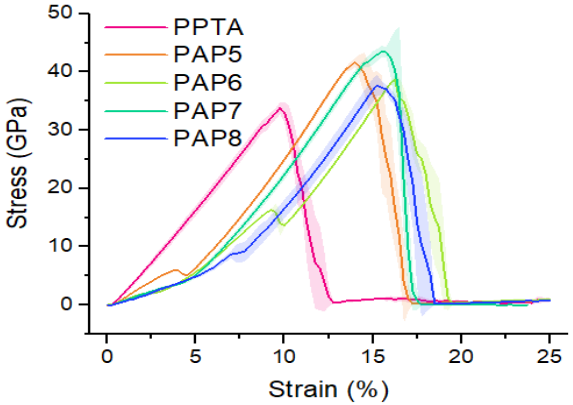
ML Models

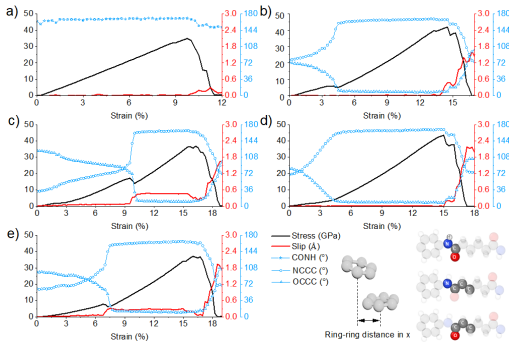
- Linear Regression
- Polynomial Regression
- Gaussian Process Regression
- Artificial Neural Network (ANN)
- Support Vector Machines (SVM)
- Deep Learning
- XGBoost

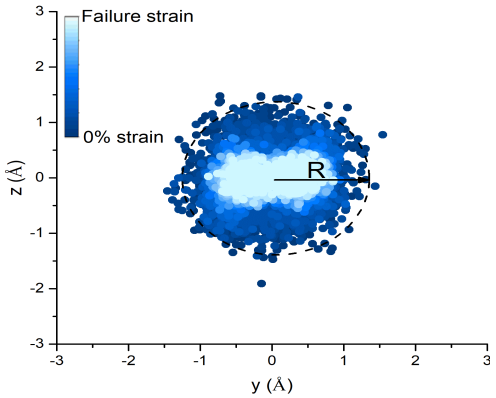
Summary of Contributions

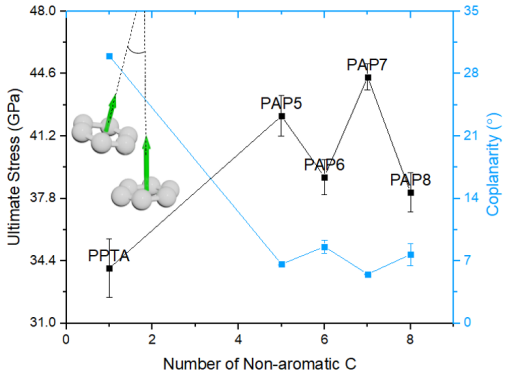
- Established a force field selection framework that can be applied to other polymeric crystals;
- Provided insight into the important fundamental question of how the processibility of high-performance polyamide PPTA can be improved by modification without compromising the mechanical properties;
- Provided new insight into how inter and intrachain interactions affect the stress-strain response at the atomic scale;
- Introduced a quantity, “waviness”, to describe the flexibility of polyamides and discovered the correlation of it with low-strain modulus
- Emphasized the critical role of the odd-even effect observed in both the elastic and ultimate properties of polyamides;
- Explained the origin of the odd-even effect by attributing it to the structure of hydrogen bonding network.

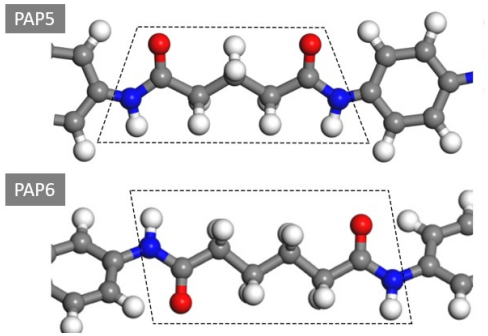












Acknowledgement

- Thanks to ExxonMobil collaborators
- Thanks to Martini Group

ExxonMobil

Dr. Spencer T. Stober

Dr. Wenjun Li

Dr. Adam B. Burns

Dr. Manesh Gopinadhan

Summary of Accomplishments (Master's & PhD):

Publications (10, including 7 first-author):
- **Journal Papers:** published (9), submitted (1)
- **Patent**: 1
- **Software Copyrights**: 3

Conferences (6):
- Presentation (4), posters (2)

Awards:
- Faculty Mentor Program Fellowship (*2022)*
- UC Merced Bobcat Fellowship (*2019, 2020, 2021, 2022)*
- Third Place Poster Award of The Web Seminar Series on Tribology (WeSST) (*2020)*
- MACES Summer Fellowship (sponsored by NASA) (2019, *2020)*
- UC Merced Travel Fellowship (*2019, 2022)*
- South China University of Technology First-tier Scholarship (2016, 2017)
- South China University of Technology Third-tier Scholarship (2015)

Peer Review Service for Journals (11):

Tribology Letters (4), Sustainability (4), Applied System Innovation (2), Applied Sciences (1)

Conference Session Chairs (2):

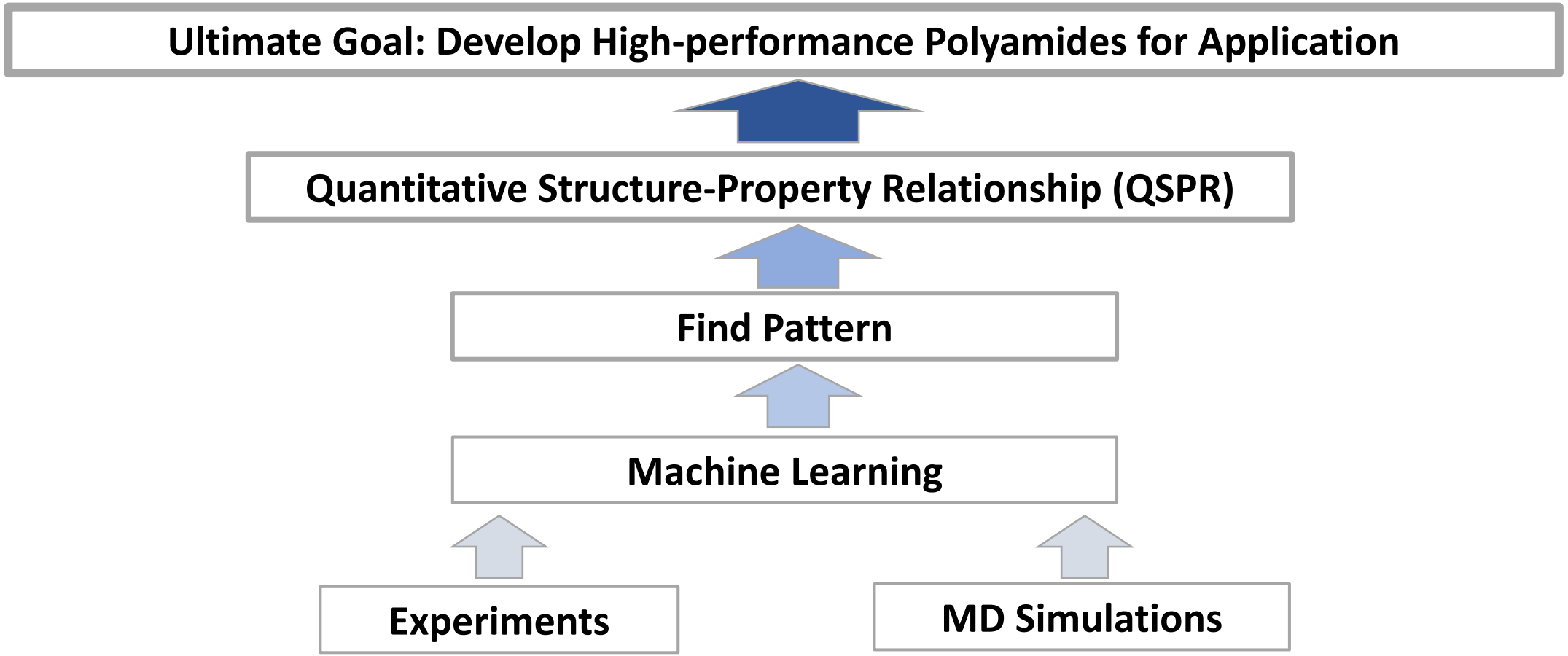
Tribochemistry and *Biotribology* sessions *at the 73rd STLE Annual Meeting & Exhibition* in Chicago 2019

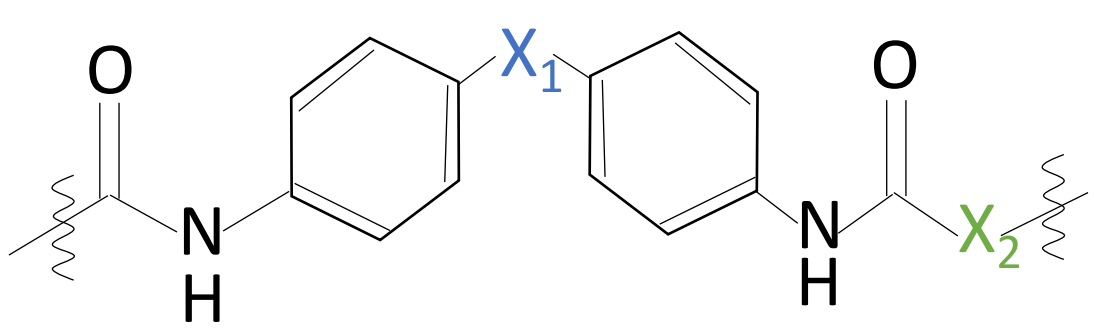
Thank you for attention!

Q & A

Appendix

Machine Learning

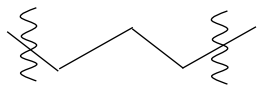




X_2:

PPTA

PAP5



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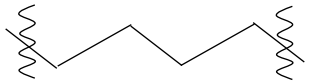

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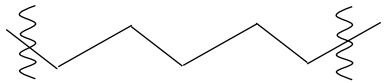

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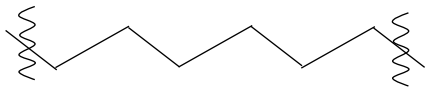
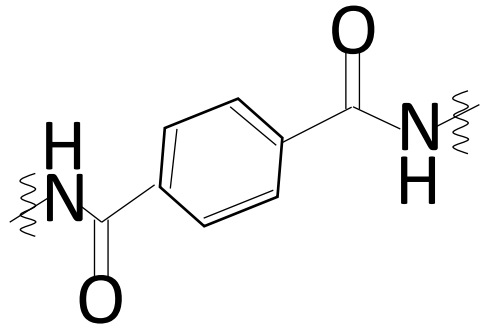


X_1:

PPTA



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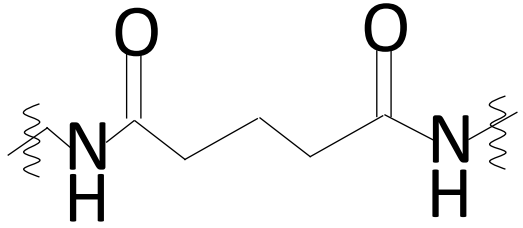

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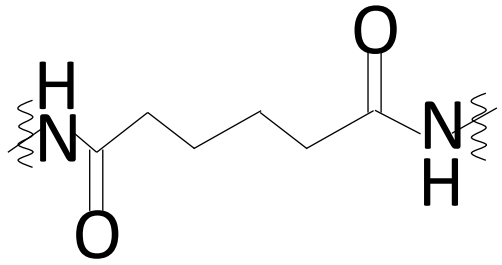

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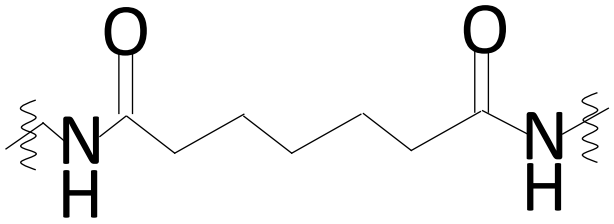

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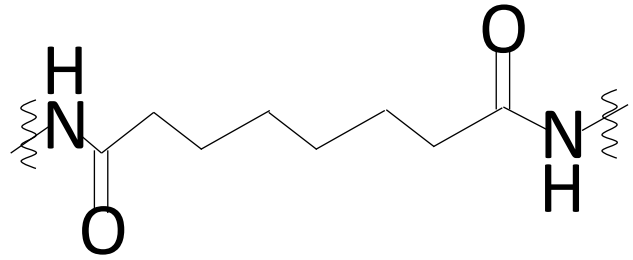
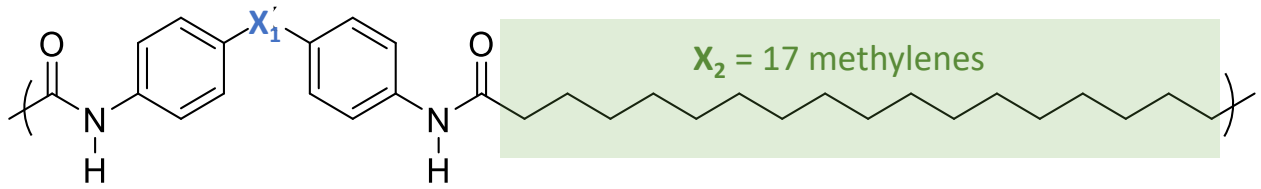
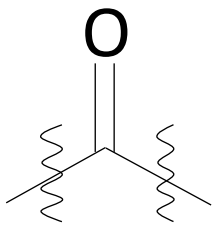
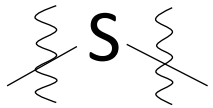
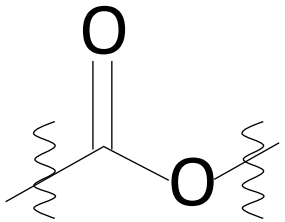
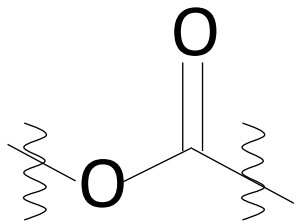
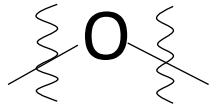
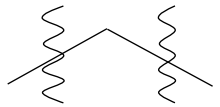
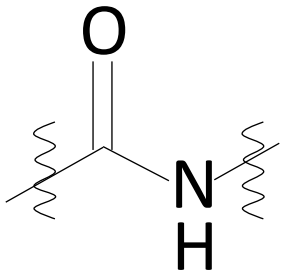
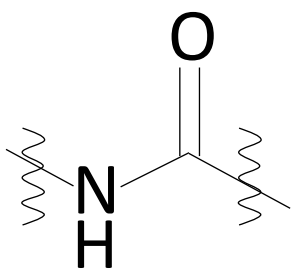
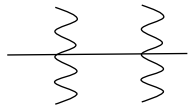
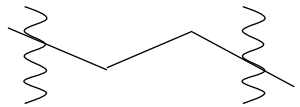
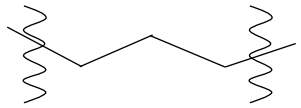
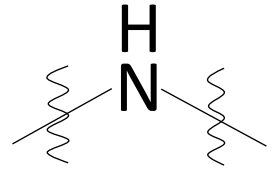




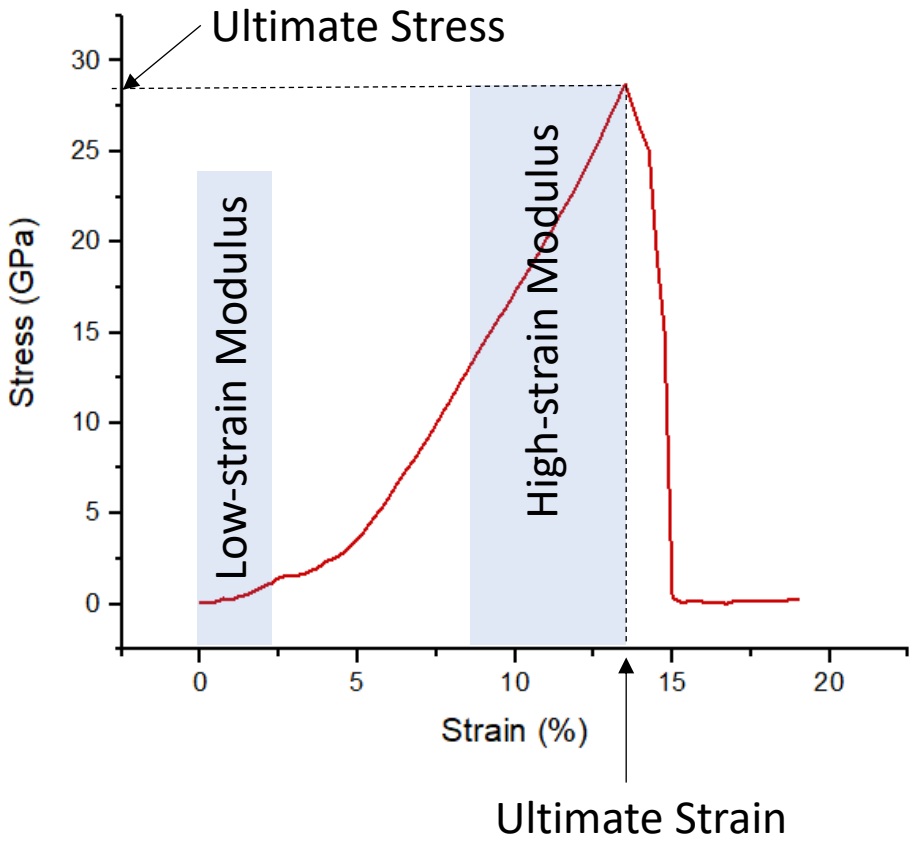
X_1:

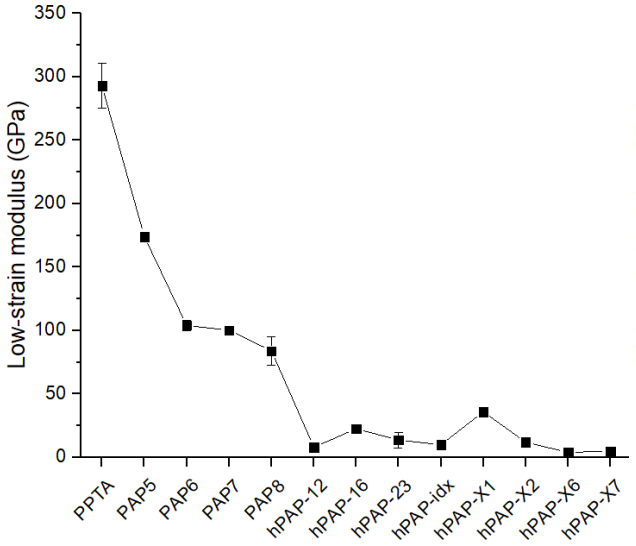
hPAP-2	hPAP-12	hPAP-14	hPAP-14-f	hPAP-16	hPAP-23
					

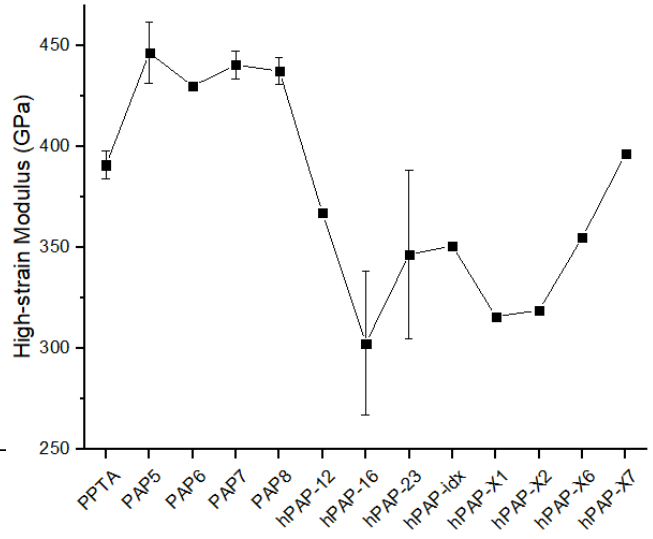
hPAP-idx1	hPAP-idx1-f	hPAP-biphenyl	hPAP-Et	hPAP-Pr	hPAP-NH
					

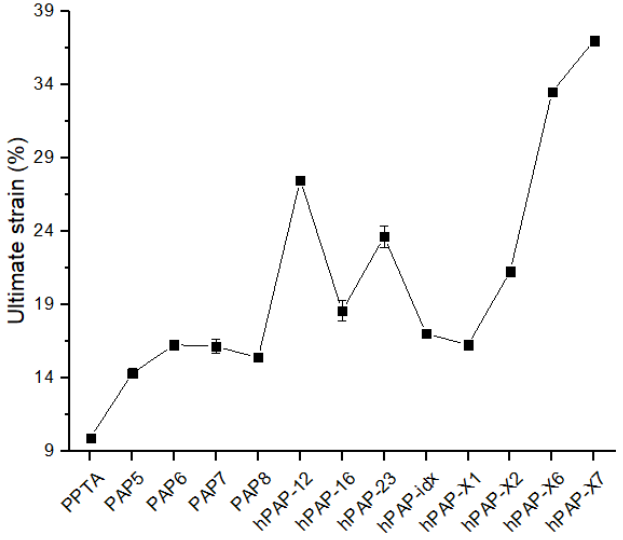
- Only part of the data is shown here

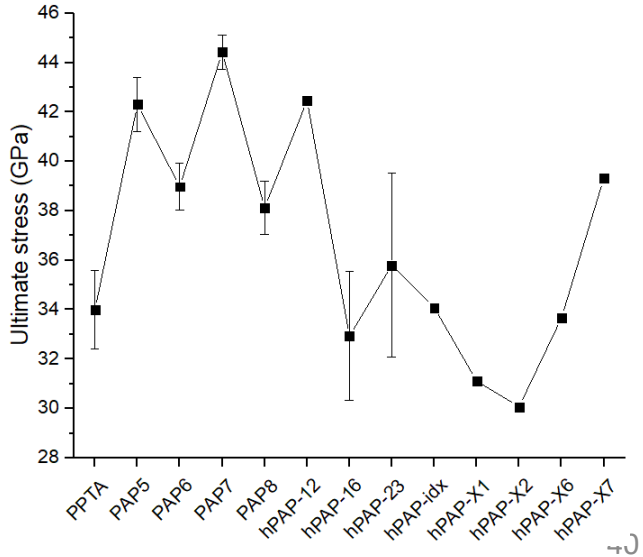
- Low-strain modulus, high-strain modulus, ultimate strain, and ultimate stress









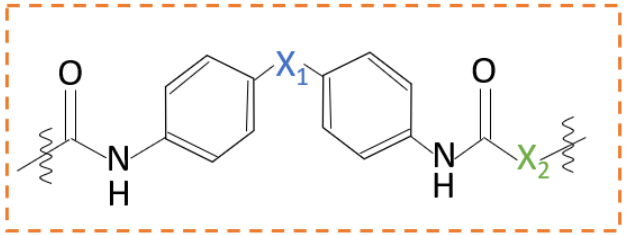


- Only part of the data is shown here

ID	Descriptor	ID	Descriptor
x_0	Equilibrium Waviness (Å)	x_9	# of O in X_2
x_1	# of Methylenes in X_1	x_10	# of C in X_2
x_2	# of Rings in X_1	x_11	a (nm)
x_3	# of S in X_1	x_12	b (nm)
x_4	# of O in X_1	x_13	c (nm)
x_5	# of C in X_1	x_14	α (°)
x_6	# of Methylenes in X_2	x_15	β (°)
x_7	# of Rings in X_2	x_16	γ (°)
x_8	# of S in X_2		

ID	Mechanical Property
y_0	Ultimate Strain (%)
y_1	Ultimate Stress (GPa)
y_2	Low-strain Modulus (GPa)
y_3	High-strain Modulus (GPa)

- For convenience, the descriptors and mechanical properties are represented as IDs (x and y)



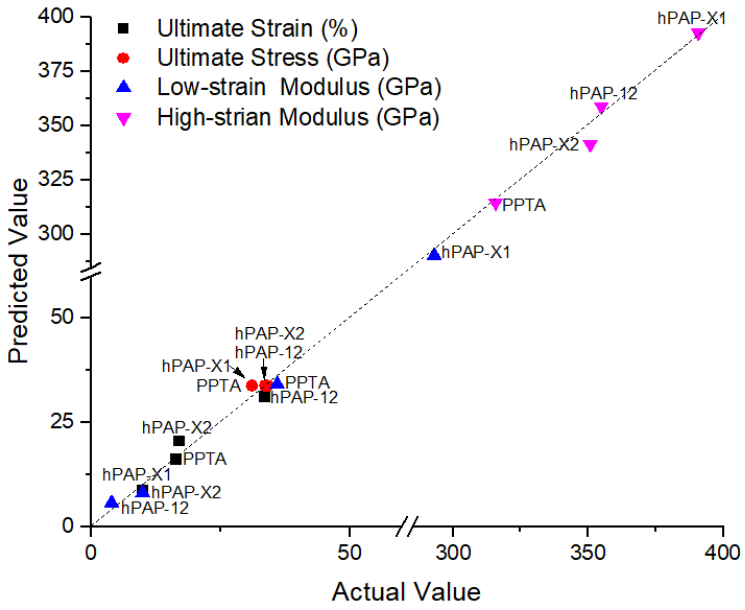
- Polynomial Regression using Scikit-Learn package in Python to predict mechanical properties of polyamides
- Tried different combinations of features (descriptors)
- Tried different degrees (1-3) of polynomial functions
- Data is separated into training set (9) and testing set (4)
- 'x_1', 'x_2', 'x_3', … 'x_14', 'x_15', 'x_16' represent the descriptors

Example of calculation results:

Descriptor Combination	Testing Set Low-strain Moduli (GPa) (hPAP-idx, PAP5, hPAP-12)	Degree of Polynomial	Root Mean Square Error (RMSE) (GPa)
Actual Value	10.0, 174.0, 8.0	-	-
['x_1']	96.5, 92.3, 96.5	1	85.6
['x_2']	60.0, 60.0, 60.0	1	77.8
…	…	…	…
['x_1', 'x_5', 'x_6', 'x_7', 'x_8']	10.6, 163.5, 10.6	1	36.7
…	…	…	…
['x_0', 'x_1', 'x_2', 'x_6', 'x_7', 'x_14', 'x_15']	10.6, 163.5, 10.6	2	1.99 ★ Best!
…	…	…	…

Training Set	PAP5	PAP7	PAP8	hPAP-12	hPAP-16	hPAP-23	hPAP-X2	hPAP-X6	hPAP-X7
Testing Set	PAP6	hPAP-X1	PPTA	hPAP-idx					

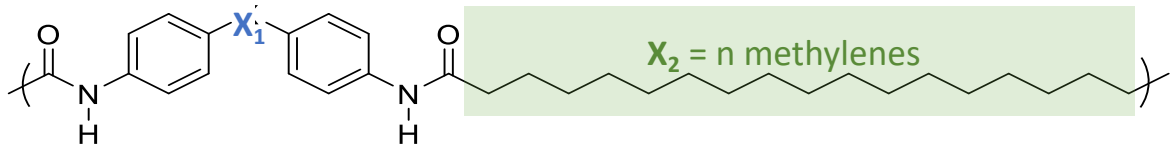
Low-strain Modulus	High-strain Modulus	Ultimate Strain	Ultimate Stress
Most Relevant Descriptors			
Equilibrium Waviness (Å)	Equilibrium Waviness (Å)	Equilibrium Waviness (Å)	# of Methylenes in X_1
# of Methylenes in X_1	# of Methylenes in X_1	# of Methylenes in X_1	# of S in X_1
# of Rings in X_1	# of C in X_2	# of Rings in X_1	
# of Methylenes in X_2	a (nm)	# of S in X_1	
# of Rings in X_2		# of Methylenes in X_2	
α (°)			
β (°)			
Root Mean Square Error of Best Model			
1.99 GPa	5.16 GPa	2.20 %	1.36 GPa
Best Model			
2nd degree polynomial	1st degree polynomial	3rd degree polynomial	2nd degree polynomial



- Four data points in each color represent four materials in the testing set

More data:

- Expanding the data pool by varying the length of methylene groups (300+ more)



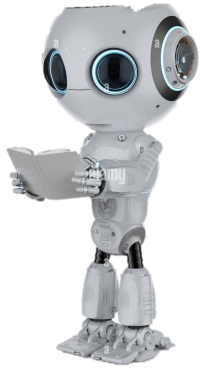
- Polyamides from literature/database (300+)

Descriptors:

- Calculate dynamics (3D) descriptors from trajectories of MD simulations by developing a Python Package [1]

Machine Learning

input



output

Mechanical Properties

- Low-strain modulus
- High-strain modulus
- Ultimate strain
- Ultimate stress

ML Models:

- Linear Regression
- Polynomial Regression
- Gaussian Process Regression
- Artificial Neural Network (ANN)
- XGBoost

[1] **Yang**, Panwar, and Martini. PyL3dMD: Python LAMMPS 3D Molecular Descriptors. (To be submitted)