Project Notes :

Project Title: Novel PLA Nanocomposite Bioplastic For Use In Packaging
Name: Raihan Ahmed

Commented [CK1]: 10/8/2024 10 full entries + 2patents

Nice job with your project notes. Keep it up.

Note Well: There are NO SHORT-cuts to reading journal articles and taking notes from them. Comprehension is paramount. You will most likely need to read it several times, so set aside enough time in your schedule.

Table of Contents

Knowledge Gaps :

This list provides a brief overview of the major knowledge gaps for this project, how they were resolved and where to find the information.

Knowledge Gap	Resolved By	Information is located	Date resolved
Structure and properties of common ordinary plastics	Reading review articles about bioplastics that go over conventional plastics.	Article #6 notes	9/20/24
What are the advantages of plastics involving nanoparticles?	A journal article about nano-particles being incorporated into PVA plastic.	Article #9 notes	9/24/24
What is the solvent casting technique, and how is it carried out?	An article that includes instructions on preparation of a plastic film.	Article #9 notes	9/24/24
What is the purpose of FTIR, and how are its results interpreted?	Article that explains where it was used	Article #9 notes	9/26/24

Literature Search Parameters:

These searches were performed between (Start Date of reading) and XX/XX/2019.
List of keywords and databases used during this project.

Database/search engine	Keywords	Summary of search
Nature.com search engine https://www.nature.com/search	Bioplastic	9/3/24 I wanted to get some sort of intro into bioplastics, so I searched on nature.com to find a high-quality paper on them. There, I found Article #3 and Article #9.
Google scholar	Bioplastic neural network Bioplastic review	9/18/24 I was interested in the computational side of bioplastics research, if it even exists, and I found article #5. 9/19/24 I wanted a general overview of bioplastics as a whole to get an idea of every topic that the field encompasses. I found articles #4 and #6.
USPTO Search	Bioplastic	10/4/24

		Patents #1 and #2 were found.

Tags:

Tag Name	
#algorithm	#Step-detection
#naive	#heuristic
#PVA	
#blend	#packaging
#review	#biomedical
#tissue engineering	#PHA
#machine learning	#computer simulation
#food packaging	#turbulence
#synthesis	#biosynthesis

#physics	#water
#chemical engineering	#PLA
#PVA	#nanoparticles
#cellulose	#MD

Article #Template Notes: Title

Article notes should be on separate sheets

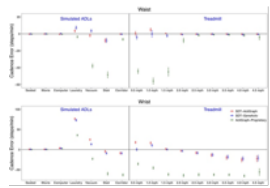
KEEP THIS BLANK AND USE AS A TEMPLATE

Source Title	
Source citation (APA Format)	
Original URL	
Source type	
Keywords	
#Tags	
Summary of key points + notes (include methodology)	
Research Question/Problem/ Need	
Important Figures	
VOCAB: (w/definition)	
Cited references to follow up on	

Follow up Questions	

Article #1 Notes: 8/22/24 – A transparent method for step detection using an acceleration threshold

Source Title	A Transparent Method for Step Detection using an Acceleration Threshold
Source citation (APA Format)	Ducharme, S. W., Lim, J., Busa, M. A., Aguiar, E. J., Moore, C. C., Schuna, J. M., Jr, Barreira, T. V., Staudenmayer, J., Chipkin, S. R., & Tudor-Locke, C. (2021). A Transparent Method for Step Detection using an Acceleration Threshold. *Journal for the measurement of physical behaviour, 4*(4), 311–320. https://doi.org/10.1123/jmpb.2021-0011
Original URL	https://doi.org/10.1123/jmpb.2021-0011
Source type	Journal Article
Keywords	physical activity monitor, accelerometer, step algorithm, physical activity, wearable devices
#Tags	#algorithm, #step-detection, #naive
Summary of key points + notes (include methodology)	In this article, researchers performed a study of 75 adults to determine an acceleration threshold for devices to detect steps while walking. Raw acceleration signals from device accelerometers were measured, and magnitude peaks above varying thresholds were counted to compare against the real step value and ascertain the optimal threshold. By minimizing error to within 2 steps/min on the waist and 6 steps/min on the wrist, the researchers thus created a robust method of characterizing step behavior.
Research Question/Problem/ Need	How can a device detect when an individual has made a step based on its accelerometer data?
Important Figures	- Error within 2.28 steps/min for waist and 6.47 steps/min for wrist

	-  Graph of error for the algorithm doing various tasks
VOCAB: (w/definition)	- AP stands for anterior-posterior, which refers to accelerometer measurements in the front-back axis. - ML stands for medial-lateral, which is accelerometer measurements in the left-right axis. - V stands for vertical, which refers to the corresponding accelerometer measurements. - VM stands for vector magnitude, the magnitude of the acceleration vector from the accelerometer. - A high pass filter removes low-frequency signals from a wave, and a low pass filter correspondingly removes high-frequency signals. - Tri-axial accelerometry (the meaning is self-evident, but it's important to consider that this is as opposed to single-axis accelerometry). - SDT stands for step detection threshold, or the threshold of VM required to measure a step. - Ambulation refers to walking.
Cited references to follow up on	1. Kraus et al., 2019, which supposedly provides an explanation of the relevance of step-counting to health, which can help motivate this project. 2. Del Din et al., 2016, which provides an alternative technique based on "continuous wavelet transforms". 3. Vaha-Ypya et al., 2018, since it uses similar methods for metrics besides step-count (that is, postural orientation).
Follow up Questions	1. How can this method of detecting steps based on simple magnitude of acceleration, be adapted to erratic movements like dancing, spinning, braking in a car, etc.? 2. How can other data, like GPS, be utilized to improve the estimation of step count? 3. How can methods like this be adapted to measure other aspects of one's stride (i.e, distance, symmetry)?

Article #2 Notes: 9/1/24 – Step Detection Algorithm for Accurate Distance Estimation Using Dynamic Step Length (summer article, read 7/10/24)

Source Title	Step detection algorithm for accurate distance estimation using dynamic step length
Source citation (APA Format)	Abadleh, A., Al-Hawari, E., Alkafaween, E., & Al-Sawalqah, H. (2017). Step detection algorithm for accurate distance estimation using dynamic step length. *18th IEEE International Conference on Mobile Data Management (MDM)*, 324-327. https://www.doi.org/10.1109/MDM.2017.52
Original URL	https://www.doi.org/10.1109/MDM.2017.52
Source type	Journal Article
Keywords	distance estimation, peaks, step length, accelerometer
#Tags	#step detection, #heuristic, #algorithm
Summary of key points + notes (include methodology)	This article provides a novel algorithm for counting steps, which is inextricably tied to counting distance travelled. To avoid the pitfalls of naively integrating the user's acceleration using the accelerometer device, since it is prone to cascading error – the article offers the alternative of multiplying a fixed step length by the number of steps. However, due to potential variance and erratic steps, dynamic step lengths must be accounted before. The algorithm begins by measuring the acceleration magnitudes over time, then using a low pass filter to reduce noise in the data. A step is detected when the signal has a peak within a certain time range. Then, to account for different types of steps, the distance is calculated by summing the peak acceleration for each step by a weight representing the relative step size compared to the average. The results were evaluated by asking volunteers to walk in a corridor at varying speeds, and in both

<table>
<tr><td></td><td>straight and winding lines. The authors find that the new algorithm greatly reduces error, even with larger distances.</td></tr>
<tr><td>Research Question/Problem/ Need</td><td>What algorithm can accurately estimate distance and steps using a device’s accelerometer data?</td></tr>
<tr><td>Important Figures</td><td>Results of the algorithm:

TABLE1. PROPOSED APPROACH RESULTS
<table>
<tr><th>Gender</th><th>Real Distance /m</th><th>Est. number of steps</th><th>Est. distance /m</th></tr>
<tr><td>Male</td><td>10</td><td>9</td><td>9.6</td></tr>
<tr><td>Male</td><td>20</td><td>19</td><td>19.5</td></tr>
<tr><td>Male</td><td>35</td><td>36</td><td>33.3</td></tr>
<tr><td>Male</td><td>100</td><td>105</td><td>103</td></tr>
<tr><td>Female</td><td>10</td><td>10</td><td>9.2</td></tr>
<tr><td>Female</td><td>20</td><td>24</td><td>23</td></tr>
<tr><td>Female</td><td>35</td><td>34</td><td>33</td></tr>
<tr><td>Female</td><td>100</td><td>101</td><td>98</td></tr>
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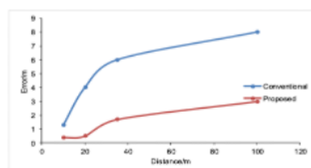

Fig. 6. The proposed approach results compared to conventional peak detection algorithm.

- Performed well compared to competing algorithms</td></tr>
<tr><td>VOCAB: (w/definition)</td><td>- PDR stands for Pedestrian Dead Reckoning. It refers to estimating location by measuring movements from a known location, possibly by doubly integrating accelerometer data.
- Kalman filter is an algorithm that reduces noise in collected data by calculating information related to it over time. (Should research this more).
- Accelerometer is a device, found in mobile phones, that measures acceleration.</td></tr>
<tr><td>Cited references to follow up on</td><td>- Liu et al., 2015, for its intriguing approach to step detection that involves neural networks.
- Abadleh et al., 2014, for an application of such an algorithm to indoor positioning – determine what step detection / distance estimation can practically be used for.
- Cho et al., 2003, for a similar reason.</td></tr>
</table>

Follow up Questions	- Clarifying question: When estimating distances, why are step sizes turned into fixed weights (0.5, 1.0, or 1.5), before adding them together? Wouldn't this just reduce accuracy? - What application does step detection and distance estimation have to indoor positioning? - How can a varying stride be predicted and accounted for by an algorithm? - How can such an algorithm be taken beyond simple handheld usage?

Article #3 Notes: 9/3/24 – New polyvinyl alcohol/gellan gum-based bioplastics with guava and chickpea extracts for food packaging

Source Title	New polyvinyl alcohol/gellan gum-based bioplastics with guava and chickpea extracts for food packaging
Source citation (APA Format)	Elsaeed, S., Zaki, E., Diab, A., Tarek, M., & Omar, W. A. (2023, December 16). New polyvinyl alcohol/gellan gum-based bioplastics with guava and chickpea extracts for food packaging. *Scientific Reports, 13*(22384). https://doi.org/10.1038/s41598-023-49756-0
Original URL	https://doi.org/10.1038/s41598-023-49756-0
Source type	Journal Article
Keywords	bioplastic, food packaging, biodegradable
#Tags	#PVA, #blend, #packaging
Summary of key points + notes (include methodology)	**Summary** In the interest of replacing traditional fossil-fuel based plastic packaging, researchers developed a bioplastic using a blend of polyvinyl alcohol, gellan gum, and chickpea and guava extract. They then tested its biodegradability, mechanical properties, and cytotoxicity, as well as various other metrics – to determine its viability, and found it excelled in all three qualifications. **Why is this important?** Regular fossil-fuel based plastics will not degrade once disposed of, and pose a threat to the environment and wildlife. A viable (strong, and having similar properties to ordinary plastics) and biodegradable alternative is needed, and bioplastics provide a path towards this. **Data** - The chemical properties of the PVA (polyvinyl alcohol)/GG (gellan gum) blends.

- The mechanical properties of the original PVA/GG film must be measured, like tensile strength, must be measured at different compositions of the components to determine the most promising one.
- Weather testing and water wettability tests
- Cytotoxicity
- Oxygen and water permeability
- LCA (Life Cycle Assessments) to measure biodegradability.
- CO2 emissions

Methods and Analysis

- The PVA/GG film was prepared with a solvent casting technique, at different compositions of each component.
- FTIR (Fourier Transform Infrared Spectroscopy) was used to characterize the PVA/GG blends chemically. **Analysis**: Looking at the different peaks on the FTIR readout can characterize how they bonded.
- A tensile tester was used to measure the mechanical properties. **Analysis:** Comparing the tensile strength of the different blends of PVA and GG, as well as the blends with guava and chickpea extract.
- Cytotoxicity was measured on kidney cells with a "MTT" protocol that is reported in other papers.
- Water vapor transmission rate (WVTR) was measured by placing the films on top of a glass water bottle in a place with 90% humidity. The decrease in weight of the bottle was measured with a balance scale, over a period of days. The WVTR is the slope of the regression line of this weight over time, per unit area. Oxygen permeability was measured similarly. **Analysis:** The permeability is calculated by dividing the mass change by exposed area and elapsed time.
- Weather testing was done with a specialized machine (Model QUV/se) in light and dark weather.
- Life cycle assessment was done using a model provided in a different paper.
- CO2 emissions were calculated based on the CO2 emissions of the individual components of the bioplastic.

Results

- The FTIR elucidated the chemical properties of the PVA/GG film.
- The stress vs. strain for each blend was determined and graphed.

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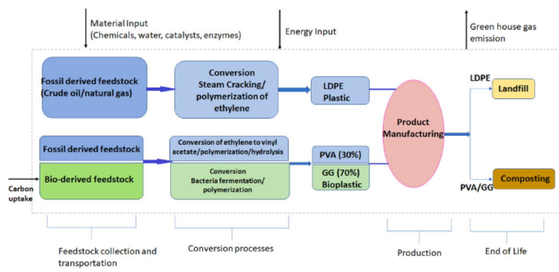
- The cytotoxicity was measured with a cell viability of 99.67%, making it very safe for food packaging.
- The WVTR was comparable to other food packaging bioplastics, while the oxygen permeability was decreased.
- The weather test exhibited harsh damage to the plastic, a good sign of its biodegradability.
- The authors proposed a life cycle assessment (LCA) but did not follow up.



-
- The PVA had an emission measurement of 5.5 kg CO_2 emissions per kg plastic. For comparison, other state of the art bioplastics has values of 2.9 and 7.8. The addition of guava and chickpea extract greatly improve this, as shown in a graph.

How does it answer the CQ?

- This analysis helps characterize the safety, biodegradability, and influence on the environment of the novel bioplastic, while ensuring that it is still mechanically viable for food packaging.

How does it impact the field?

- The authors have proved that blending biomass with synthetic bioplastics can greatly reduce CO_2 emissions. Thus bioplastics are a viable solution to the issues with fossil plastics.

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<td>Research Question/Problem/ Need</td>
<td>Do bioplastics based on polyvinyl alcohol/gellan gum, combined with chickpea and guava extracts, have strong mechanical and thermal properties, as well as being safe and biodegradable?</td>
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Important Figures

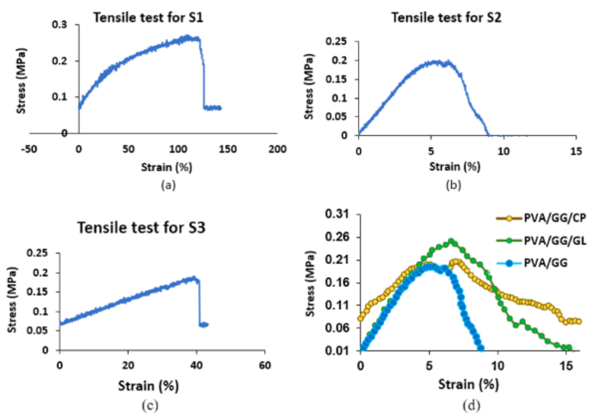


Figure 5. The tensile strength measurement for (**a**) sample S1, (**b**) sample S2, (**c**) sample S3 and (d) S2, S2/CP and S2/GL.

S2 performed best in the tensile test (30/70% PVA/GG).

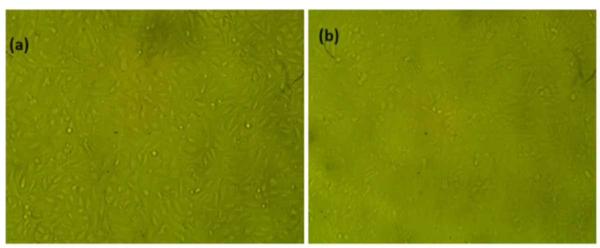
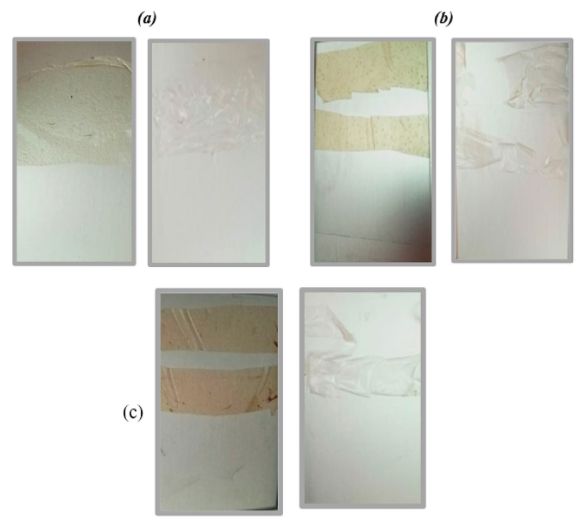


Figure 7. (**a**) Control Vero cells and (**b**) Effect of PVA/GG (S2) on cell viability of Vero normal cell line at concentration 1000 uL and incubation time 24 h.

Little to no effect on cell viability.

	 **Figure 9.** Accelerated weathering test, (**a**) PVA/GG (S2), (**b**) S2 with GL extract and (**c**) S2 with CP extract. Demonstrated adequate degradation in accelerated weather test.
VOCAB: (w/definition)	- PVA = Polyvinyl alcohol, a polymer that's water-soluble, synthetic, and biodegradable. - GG = Gellan gum, a natural polysaccharide - FTIR = Fourier transform infrared spectroscopy – a tool that obtains absorption data over the infrared spectrum, which internally uses the mathematical concept of the Fourier transform. Used in chemistry for identifying compounds. - Desiccator = a sealed container for moisture-sensitive chemicals - WVTR = Water vapor transmission rate - LCA = Life cycle assessment, a qualitative assessment to determine the impact of the bioplastic on the environment
Cited references to follow up on	- Texira et al., 2023, for the application of PVA to tissue engineering. - Sudhamani et al., 2003 – an article almost solely focused on FTIR, which could provide useful information about it. It also is cited as a reference for the solvent casting technique. - Benavides et al., 2020, for an example of a life-cycle assessment.

Follow up Questions	- What is the solvent casting technique, and how is it carried out? - What is the purpose of FTIR, and how are its results interpreted? - Which other polymers can serve as a base for a blend with other plastics? - Which other natural products produce a viable and useful bioplastic when blended with PVA? - How does the blending of these polymers affect the chemical properties and biodegradability of the resultant polymer? - How can these concepts be applied to tissue engineering?

Article #4 Notes: 9/15/24 – Innovations in applications and prospects of bioplastics and biopolymers: a review

Article notes should be on separate sheets

Source Title	Innovations in applications and prospects of bioplastics and biopolymers: a review
Source citation (APA Format)	Nanda, S., Patra, B. R., Patel, R., Bakos, J., & Dalai, A. K. (2022). Innovations in applications and prospects of bioplastics and biopolymers: a review. *Environ Chem Lett, 20*(1), 379-395. https://doi.org/10.1007/s10311-021-01334-4
Original URL	https://doi.org/10.1007/s10311-021-01334-4
Source type	Journal Article
Keywords	Biodegradability, bioplastics, polymers
#Tags	#review
Summary of key points + notes (include methodology)	- This is a review article, so no methodology. - **Summary –** It goes over the drawbacks of existing plastics, then introduces a set of candidate bioplastics, which are PHA, Polylactic acid, Poly-3-hydroxybutyrate, polyamide 11, polyhydroxyurethanes, and various plastics based on cellulose, starch, proteins, and lipids. It finishes with some challenges regarding these bioplastics. Notes - **Why is it important?** Non-biodegradable plastics are detrimental to the environment, and the microplastics that remain are harmful to human health. A viable alternative is necessary to eliminate these concerns. - (The intro of the article goes over essentially every problem with traditional plastics – this is not the best source for that so I basically glossed over it). - **Definition of bioplastic** – Confusing, but it means either bio-based or biodegradable. - Bioplastics degrade after 3-6 months.

	- Degradation can occur under controlled environ. / Humid conditions – **ASTM and ISO have standardized tests to measure this.**
	- **PHA**
	    o synthesized naturally by bacteria to store energy and carbon.
	    o Contains an –R group which may vary.
	    o Used medically/industrially, many biomedical applications.
	    o Very non-toxic
	    o Thermoplastic
	- **PLA (Polylactic acid)**
	    o Composed of lactides
	    o Easy to synthesize, not toxic, beneficial mechanical properties.
	    o Releases organic compounds on degradation which can be utilized by plants.
	    o Used for packaging, some development working on varying the chemical structure.
	- **Poly-3-hydroxybutyrate**
	    o A PHA synthesized by fermentation.
	    o Very good mechanical properties like melting temp., tensile strength, etc., which resemble those of many traditional plastics.
	    o Used for surgical implants and packaging.
	    o Impractical production cost.
	- **Polyamide 11**
	    o Belongs to nylon family.
	    o Produced from bio-based sources.
	    o Non-biodegradable but low-environmental impact.
	- **Polyhydroxyurethanes**
	    o Alternative to polyurethanes, which cause extreme pollution.
	    o Beneficial mechanical properties for adhesives.
	- **Cellulose-based**
	    o Biodegradable, durable, stiff.
	    o Fast degradation.
	    o Blending with other polysaccharides can improve mechanical properties.
	    o Commonly used in packaging.
	- **Starch-based**

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Very affordable
Abundant, but high odor which must be studied.
Essential oils can benefit antimicrobial properties (sounds like a scam but I guess it's true).
Sensitive to moisture and mechanical properties are awful but can be improved by blending with other polymers.
- Protein-based
Can have great mechanical properties, widely used.
- Lipids
Useful in food-packaging for hydrophobicity.
Challenges
- Controlled conditions required for degradation
- Cost competitiveness
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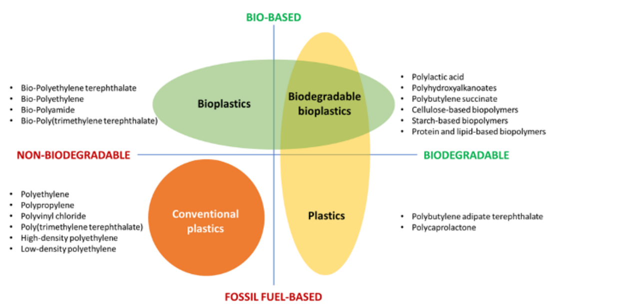
<tr><td>Research Question/Problem/ Need</td><td>What are benefits, applications, and considerations related to bioplastics and their chemistry?</td></tr>
<tr><td>Important Figures</td><td>


This provides a guide to the distinction between bio-based, biodegradable, and bioplastics – as well as including prominent examples.
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<tr><td>VOCAB: (w/definition)</td><td>
- Elastomeric – regaining original shape when deformed.
- Thermoplastic – plastic that becomes moldable with heat.
- PHA – Polyhydroxyalkanoate – Biodegradable plastics that occur naturally and are synthesized by microorganisms.
</td></tr>
<tr><td>Cited references to follow up on</td><td>
- ASTM, 2021 and ISO, 2018, to investigate testing of biodegradation.
- Ray & Kalia, 2017, to see how PHA has been applied to tissue engineering.
</td></tr>
</table>

	- Osorio et al., 2019, to read about the odor problems present with starch bioplastics. - Calva-Estrada et al., 2019, for a review on protein-based bioplastics, to assess their benefits and drawbacks.
Follow up Questions	- How cost-competitive are PHAs with conventional plastics? - How is degradation tested, and what are some issues with this methodology? - What are biomedical applications of PHAs? - Why are protein-based bioplastics not widely adopted?

Article #5 Notes: 9/19/24 – Bioplastic design using multitask deep neural networks

Source Title	Bioplastic design using multitask deep neural networks
Source citation (APA Format)	Kuenneth, C., Lalonde, J., Marrone, B. L., Iverson, C. N., Ramprasad, R., & Pilania, G. (2022, December 3). Bioplastic design using multitask deep neural networks. *Communications Materials, 3*(96). https://doi.org/10.1038/s43246-022-00319-2
Original URL	https://doi.org/10.1038/s43246-022-00319-2
Source type	Journal Article
Keywords	bioplastic, food packaging, biodegradable, machine learning
#Tags	#PHA, #machine learning, #computer simulation, #packaging
Summary of key points + notes (include methodology)	**Summary** Researchers used publicly available data on polymers to train a machine learning model on different modifications to the bioplastic PHA, to find candidate polymers to replace common conventional plastics. After developing their model, a nearest neighbor search was able to find candidate polymers, with predicted properties similar to the target plastics. **Why is this important?** Non-biodegradable plastic waste is harmful to the environment, threatening ecosystems and humans, so a biodegradable yet functional alternative must be developed. **Notes:** - Plastic is harmful to the environment, microplastics are harmful to humans. - PHA is important because it can easily be made by microorganisms from industrial sources. - Mechanical properties can easily be modified in PHA. - Important properties (verbatim from paper) “Young’s modulus, tensile strength, elongation, glass transition

	temperature, melting temperature, and degradation temperature."
	- Lots of possible modifications
	  o # of carbons in main chain
	  o # of carbons in side chain
	  o Functional group of side chain
	- For ideal mechanical properties + melting temp and degradation temp, make copolymer with conventional plastic.
	- Food industry needs plastics with low gas permeability.
	- Search space is too large (millions) for experimentation, and even for molecular simulation.
	- 23,000 data points from experiments => multitask deep neural network that predicts the same properties for the candidate plastics.
	- List of properties (taken directly from paper):
	  o Thermal (glass transition temp., melting temp., degradation temp.)
	  o Mechanical (Young's modulus, tensile strength at yield/break, elongation)
	  o O_2, CO_2, N_2, H_2, He, CH_4 permeability
	- 540 PHAs + 13 conventional polymers => 1.4 million candidates
	- Polymer data taken from the PoLyInfo repository (**only used data points collected with the same methods**), scaled to [0,1]
	- DBSCAN clustering algorithm to eliminate outliers
	- Multitask DNN (deep neural network) is most effective at finding correlations.
	- Three multiproperty predictors, for 13 total properties
	- Very high R^2 (0.97/0.93) for meta-learner and cross-validation, improvement over previous research
	- **Candidate creation –** 540 PHAs from 1-6 carbons in main and side chain, 17 diff. function groups. 13 conventional polymers from list of most common.
	- Each polymer can be turned into a fingerprint using SMILES (Simplified molecular input line entry system) strings.
	  o From there, transformed into 849 component vectors by incorporating information from 3 length scales: atomic fragments, then QSPR (quantitative structure property relationship) fingerprints using the software RDKit, and then large-scale morphological properties
	  o Individual fingerprints consolidated into final fingerprint vector.

	◦ No physical interpretation of the vector - Researchers used 2D UMAP (Uniform manifold approximations and projections) to visualize the fingerprint, determined that it accurately represented the space of polymers. ◦ Found glass transition temp. is positively correlated with melting temp. and Young's modulus at room temp. ◦ Tensile strength at break is positively correlated w/ Young's modulus. ◦ Linear correlation of O2 and CO2 permeability - Now they need to determine optimal replacement for 7 common plastics. ◦ Nearest neighbor search within each subgroup of copolymers ◦ Used Scikit-learn. ◦ Next, used intuition to determine best replacement from candidates. - The 7 plastics' properties are within the property distribution for the search space – however, difficult to find replacements, since these plastics tend to be at the extreme of the distribution. - Every bio-replacement contains aromatic group (involving benzene). - **Synthesis** ◦ Can easily be biosynthesized – example of PHAs with nitrophenyl groups synthesized by bacterium *Pseudomonas oleovorans.* ◦ Gene editing/Crispr also has potential. ◦ Can possibly be chemically synthesized. - Limitations with respect to manufacturing & morphology, many properties are not taken into account – informatics pipeline must be updated
Research Question/Problem/ Need	Which polyhydroxyalkanoate (PHA) based plastic serves as the most effective replacement to seven common non-biodegradable, petroleum-based plastics?

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<td>Important Figures</td>
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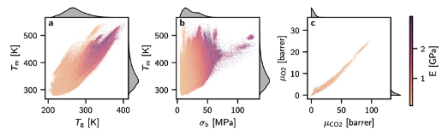
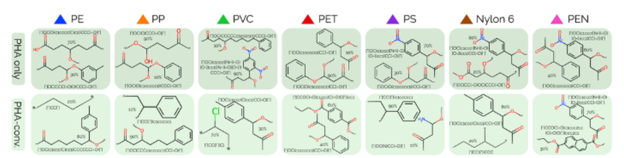


Fig. 3 Property relations of almost 1.4 million bioplastic candidates. T_m, T_g, σ_b, μ_{O_2}, μ_{CO_2}, and E in the panels a–c stand for melting temperature, glass transition temperature, tensile strength at break, O_2 gas permeability, CO_2 gas permeability, and Young's modulus, respectively. The data point densities are indicated in the plot margins.

Relationships between certain properties of bioplastics. Could be useful for further research.



The candidate polymers – note the benzene in every picture.

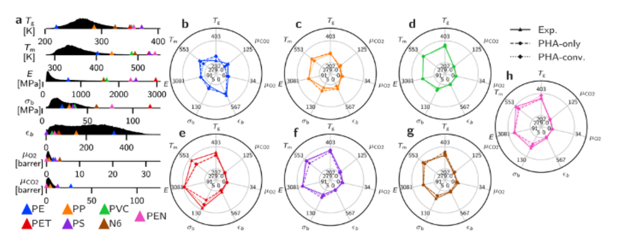


Fig. 5 Experimental and predicted properties. a Property density profiles computed over the entire prediction set of bioplastic candidates. Missing x-axes beyond a certain cutoff indicate zero predicted property densities over those property ranges. The triangles show experimental properties of the seven commodity plastics. Full polymer names are listed in Table 3. b–h Property radar charts for each commodity plastic. Triangles with solid lines show the experimental properties. Circles with dashed lines and diamonds with dotted lines indicate predicted properties of the bio-replacements in Fig. 4 for the copolymer subgroups of PHA-only and PHA-conventional polymers, respectively.

The experimental properties of the existing fossil plastics vs. the neural network predicted properties of the candidate bioplastics. They match relatively well.
</td>
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<tr>
<td>VOCAB: (w/definition)</td>
<td>
- PHA = polyhydroxyalkanoate, a family of plastics that can be synthesized by microorganisms
- MD = molecular dynamics, which entails computer simulations of the actual movements of atoms and molecules
- Multitask neural network = a neural network trained to perform multiple tasks by taking advantage of their similarities.
- Elongation = deformation of a material when force is applied
</td>
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</table>

	- Copolymer = Multiple types of polymers linked together - Homopolymer = the same type of polymer linked together - Informatics = study of information - UMAP = uniform manifold approximations and projection – a tool to visualize the multi-dimensional data often encountered in ML - Morphology = study of the structure of a compound
Cited references to follow up on	- Naser et al., 2021, for info on PHA synthesis. - Weininger, 1998, for explanation of SMILES. - Zhong, 2021, for overview of ML usage in science & engineering. - Kuenneth, 2021, for information on multitask learning with respect to polymers.

Follow up Questions	- Which other polymers can be used as a base for a similar experiment?
	- How do these candidate plastics perform experimentally?
	- What would the cost of biosynthesis be, and how would it fare relative to ordinary chemical synthesis?
	- **Knowledge gaps**
	  o How does biosynthesis of plastics work?
	  o How are chemical compounds represented with "fingerprints" for processing?
	  o Why was a multitask DNN used? How do they work?

Article #6 Notes: 9/20/24 – Recent Advances in Bioplastics: Application and Biodegradation

Article notes should be on separate sheets

Source Title	Recent Advances in Bioplastics: Application and Biodegradation
Source citation (APA Format)	Narancic, T., Cerrone, F., Beagan, N., & O'Connor, K. E. (2020). Recent Advances in Bioplastics: Application and Biodegradation. *Polymers*, *12*(4), 920. https://doi.org/10.3390/polym12040920
Original URL	https://doi.org/10.3390/polym12040920
Source type	Journal Article
Keywords	Polymers, bioplastics, sustainability
#Tags	#Biomedical, #review
Summary of key points + notes (include methodology)	- Review article, so no methodology - **Summary:** This article goes over many pertinent areas of research relating to bioplastics, exploring the most promising groups of bioplastics, such as PHAs and starch-based ones, and focusing mainly on the biomedical applications of these plastics, specifically to tissue engineering and drug delivery. **Why is this important?** - Not only do conventional plastics cause pollution, harming the environment – but the alternative bioplastics also are competitive in various biomedical applications. **PHA** - Biodegradable, created by bacteria for a stress response. - Classified by length of monomer's carbon chain. **PLA** - Extremely popular, synthesized by fermentation. - Degrades slowly in soil and water. **Starch** - Plasticizers needed to improve thermal properties. - Possible to improve by blending with other biodegradable polymers. **Cellulose** - Current research is on "nanocellulose."

	Applications
	- **Drug delivery**
	    o PHA has been used in nanoparticles to facilitate drug-delivery applications.
	    o Using PLA nanoparticles exhibited improved efficacy for certain drugs over delivery without nanoparticles.
	    o A niche bioplastic, Poly-γ-glutamate acid, has been assessed to protect a drug against immunogenic antibodies.
	    o DDS based on polymers is beneficial since modifications can be introduced easily.
	- **Tissue Engineering**
	    o Bio-based materials cause immune response, bioplastics may not.
	    o PLA scaffolds helped bone growth in vitro – composite with minerals helps further with bone growth.
	    o Different bioplastics are beneficial for different types of tissue.
	    o Renal cells in PLA scaffolds helped recover blood vessels in mice.
	    o More biodegradable, but mechanical properties are lacking for bioplastics.
	- **Packaging**
	    o Starch must be modified chemically or physically for properties for viable packaging.
	    o PVA-starch blends perform well since they form H-bonds.
	    o PLA is brittle, low heat-tolerance. Needs increased mol. weight to counteract these factors.
	    o PHAs have high production cost.
	- **3D Printing**
	    o PLA is popular due to low melting point.

Research Question/Problem/ Need	This review article explores the usage of bioplastics in biomedical applications and in packaging.

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<tr>
<td>Important Figures</td>
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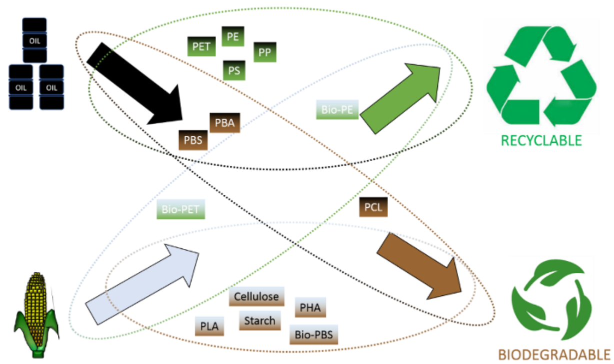

Figure 1. Four-way diagram of origin vs. end-of-life management for different polymers. Polymers originating from fossil fuels (polyethylene terephthalate (PET), polyethylene (PE), polystyrene (PS), polypropylene (PP)), or from renewable resource(s) (polybutylene succinate (PBS), polybutylene adipate (PBA), polycaprolactone (PCL)) can either be recycled or biodegraded. Biobased polyethylene terephthalate bio-PET and biobased polyethylene bio-PE are made from renewable resources and are recyclable. Polylactic acid, PLA; polyhydroxyalkanoates, PHA; biobased polybutylene succinate Bio-PBS are made from renewable resources and are biodegradable. Adapted from Emadian et al. 2017 and Narancic et al. 2018 [1,35].
A consideration of what happens to different types of plastics at the end of their lifecycle, as well as the distinction between different types of bioplastics.
</td>
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<tr>
<td>VOCAB: (w/definition)</td>
<td>PHB = Poly-3-hydroxybutyrate, a special type of PHA.
PE = polyethylene, PS = polystyrene, PP = polypropylene – all popular conventional plastics.
Nanocellulose = cellulose fibers whose hierarchical structures have been broken down to form nano-sized particles.
Immunogenic = A substance that induces an immune response.
Osteogenesis = Bone formation.</td>
</tr>
<tr>
<td>Cited references to follow up on</td>
<td>- Dassanayake et al., 2018, to investigate the practicality and usage of nanocellulose.
- Sadtler et al., 2016, to explain the benefits and drawbacks of utilizing biomaterials for tissue engineering applications.
- Lih et al., 2016, because it is an example of bioplastic-based tissue generation being done in vivo.
- Tian et al., 2017, because it investigates starch blends with PVA, which is a potentially interesting topic.
- Standau et al., 2019, for an exploration of chemical modifications of PLA.</td>
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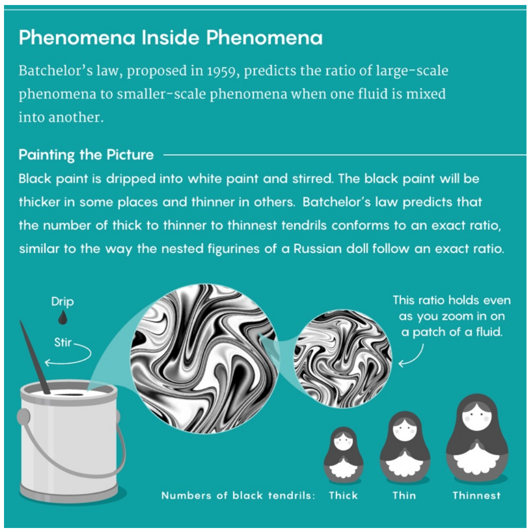
</table>

Follow up Questions	- What advantage do PHAs pose for drug delivery systems that other polymers do not? - What is the limiting factor in the high production cost of PHAs? - What mechanical properties are necessary to make bioplastics viable for tissue engineering? - Which blends of starch plastics have the most desirable properties for food packaging? - **Knowledge Gap** – What is nanocellulose, and what are the advantages of plastics involving nanoparticles?

Article #7 Notes: 9/24/24 (summer article, read 7/10/24) – Mathematicians prove universal law of turbulence

Article notes should be on separate sheets

Source Title	Mathematicians prove universal law of turbulence
Source citation (APA Format)	Hartnett, K. (2021, September 10). *Mathematicians prove universal law of turbulence.* Quanta Magazine. https://www.quantamagazine.org/mathematicians-prove-universal-law-of-turbulence-20200204
Original URL	https://www.quantamagazine.org/mathematicians-prove-universal-law-of-turbulence-20200204/
Source type	Science News Article
Keywords	Turbulence, mathematical physics, fluid dynamics
#Tags	#Turbulence, #physics
Summary of key points + notes (include methodology)	Currently, planes can only predict a narrow majority of turbulence before it occurs through weather radar, so a more sophisticated detection system is necessary. The article laments that the nature of fluids moving in different directions is hard to express in precise mathematical terms – leaving turbulence as an unsolved problem in mathematics –, but researchers have undergone a large step towards this goal, by proving a law called Batchelor's law. Fluids often form very turbulent systems – for example, when someone sprays water into a sink, it's not until a very small scale that particles near each other move in the same direction. An important problem related to turbulence is pinning down passive scalar turbulence – or how some scalar property varies along a fluid and changes with its flow. An example of this is temperature in moving sea water. Batchelor's law itself claims that the ratio of smaller scale passive scalar flow to larger scale is constant. **Methods:** The researchers used the lens of randomness to prove this theorem, since it allows them to focus on high level concepts when the specifics don't matter. **Results:** They showed that counterexamples to Batchelor's law do not exist – for example, a permanent whirlpool in water would violate this law – yet it is not possible for one to form. Later, they showed that fluids mix in a chaotic, or random fashion which eliminates all counterexamples to Batchelor's law. While this law is most likely more abstract, and not completely relevant to turbulence in airplanes, it

	suffices as a starting point to comprehend mathematically why it occurs.
Research Question/Problem/ Need	Use a mathematical model to prove a theorem about turbulence (Batchelor's law).
Important Figures	 This diagram tries to explain what the meaning of Batchelor's law is, by forming a correspondence with an easily imaginable analogy – black paint on white paint. The "black paint" is simply any scalar field on the liquid's surface, for which this theorem must be true.
VOCAB: (w/definition)	Turbulence – When the velocity of a fluid varies greatly at each point. Passive scalar turbulence – The study of turbulence with respect to phenomenon on each point on the surface of the fluid – i.e. a scalar field. Batchelor's law – Large scale and small scale phenomena on a scalar field on a fluid's surface are proportional.
Cited references to follow up on	- Bedrossian et al., 2020, since this is the actual paper with the proof, which is bound to contain more information on the important and solution to this problem. - Hartnett, K.(2019, July 9). *How Randomness Can Make Math Easier.* Quanta Magazine. https://www.quantamagazine.org/how-randomness-can-make-math-easier-20190709/

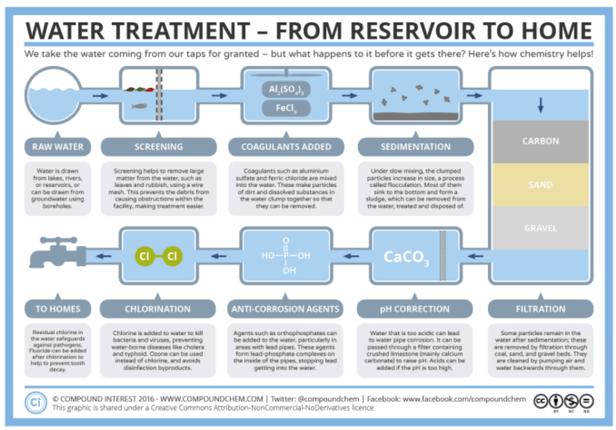
	- which describes how randomness can be used to solve mathematical problems.
Follow up Questions	- Can Batchelor's law be used to investigate the cause and prevention of turbulence? - How well does this mathematical law apply perfectly to real world physics, and are there qualifications? - How can small-scale and large-scale phenomena on a fluid be concretely defined?

Article #8 Notes: 9/24/24 (summer article, read 8/10/24) – The chemistry behind your home's water supply

Article notes should be on separate sheets

Source Title	The chemistry behind your home's water supply
Source citation (APA Format)	Brunning, A. (2016, April 21). *The chemistry behind your home's water supply.* Compound Interest. https://www.compoundchem.com/2016/04/21/water-treatment/
Original URL	https://www.compoundchem.com/2016/04/21/water-treatment/
Source type	Science News Article
Keywords	Water filtration, water purity, chemical engineering
#Tags	#Water, #chemical engineering
Summary of key points + notes (include methodology)	People around the world face difficulties with accessing clean water and providing a cheap solution to this issue is a popular issue for engineers and researchers around the globe. The article starts by stating that groundwater is generally purer than water from other sources, which could be a potential boon for a solution to this issue. Large bits of waste are removed from water through a process called "screening," which is essentially a sieve to remove large pieces. However, the article says that dissolved substances must be removed via chemicals called coagulants. Two examples are aluminum sulfate and iron (II) chloride. These neutralize negatively charged ions in the water, allowing them to clump together instead of repelling, and thus be screened. This process is called flocculation. Now, the residue forms a "sludge" which is mostly metal hydroxides and can potentially be used as fertilizer. The water is then filtered further with sand and gravel/charcoal to remove additional material. Next, acidity must be reduced by putting the water through calcium carbonate, a base. After this, to prevent the water from corroding pipes and allowing harmful metals to join in, phosphoric acid is added. Even after all of this, if there are still pathogens inside the water, it must be disinfected. This is obviously done with chlorine, which easily destroys cell walls and other organic material through oxidation. The downside is that some of the products can be carcinogens. Evidently this article does

<table>
<tr><td></td><td>not offer any novel solutions but gives a broad overview of the hurdles that must be overcome with respect to water safety.

Methodology/Results: None because this article is a general reference for water filtration.</td></tr>
<tr><td>**Research Question/Problem/ Need**</td><td>Explain the impurities that exist within water, and the most common methods of mitigating them that are applied in the real world.</td></tr>
<tr><td>**Important Figures**</td><td>


This diagram – the only one in the article – is simply a graphical representation of the article's content. However, it provides a visual representation that may be easier to follow due to an ability to track the progress of the water.</td></tr>
<tr><td>**VOCAB: (w/definition)**</td><td>Groundwater – Water that exists below the surface of the earth.
Screening – Removing larger pieces of impurities from water.
Flocculation – Chemical methods of adding coagulants to clump impurities together within water.
Trihalomethanes – Carcinogenic compounds that may form after impurities in water react with Chlorine.</td></tr>
<tr><td>**Cited references to follow up on**</td><td>- Brunning, A. (2016, April 21). *The chemistry of Limescale.* Compound Interest. https://www.compoundchem.com/2016/03/02/limescale/
- For a deep dive into minerals that can affect the purity of water.</td></tr>
</table>

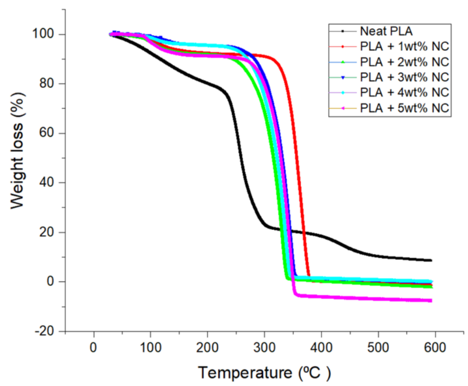
	- Brunning, A. (2016, April 21). *Fluoride & Water Fluoridation – An Undeserved Reputation?* Compound Interest. - https://www.compoundchem.com/2014/07/22/fluoride/ - For an investigation of the necessity of using fluorine in water filtration systems, which can be informative.
Follow up Questions	- How does the source of water (groundwater vs. other) impact the treatment process? - Does water treatment create any harmful byproducts for the environment or for humans? - What alternatives exist for chlorine for disinfecting water while it is being filtered?

Article #9 Notes: 9/24/24 – Thermomechanical characterization of bioplastic flms produced using a combination of polylactic acid and bionano calcium carbonate

Article notes should be on separate sheets

Source Title	Thermomechanical characterization of bioplastic flms produced using a combination of polylactic acid and bionano calcium carbonate
Source citation (APA Format)	Gbadeyan, O. J., Linganiso, L. Z., & Deenadayalu, N. (2022, June 18). Thermomechanical characterization of bioplastic films produced using a combination of polylactic acid and bionano calcium carbonate. *Sci Rep, 12*(15538). https://doi.org/10.1038/s41598-022-20004-1
Original URL	https://doi.org/10.1038/s41598-022-20004-1
Source type	Journal Article
Keywords	bioplastic, food packaging, biodegradable
#Tags	#PLA, #blend, #packaging, #nanoparticles
Summary of key points + notes (include methodology)	**Summary** Researchers synthesized a blend of the common bioplastic PLA with nano-particles of bio-based calcium carbonate, in the interest of improving its mechanical properties. Using a universal testing machine, they elucidated that it exhibited improved thermal stability, stiffness, and storage modulus. **Why is this important?** Regular fossil-fuel based plastics will not degrade once disposed of, and pose a threat to the environment and wildlife. As global plastic demand increases, a viable (strong, and having similar properties to ordinary plastics) and biodegradable alternative is needed, and bioplastics provide a path towards this. - PLA good because can form films well, and biodegradable, non-toxic, good strength. - Problems with PLA: bad thermal resistance

	- Must be improved with nanofiller - Nanoparticle => better strength, $CaCO_3$ and cellulose are promising - Right now, not synthesized from biomass – **creating $CaCO_3$ nanoparticles from *Achatina Fulica* snail shells to improve mechanical/thermal properties of PLA** **Data** - The chemical properties of the plastic blend. - The thermomechanical properties of the compound bioplastic (listed in paper) - Weather testing and water wettability tests - Cytotoxicity - Oxygen and water permeability - LCA (Life Cycle Assessments) to measure biodegradability. - CO_2 emissions **Methods and Results** - The plastic film was prepared with a solvent casting method, consolidating the nano-$CaCO_3$ solution into the PLA pellets at concentrations of 1-5%. - The researchers performed an FTIR analysis of the plastic at the different loading ratios. The FTIR elucidated the chemical properties of the film. - Thermal properties were elucidated using a thermal gravimetric analysis machine. The plastics with nano-$CaCO_3$ had improved thermal properties, degrading at higher temperatures. - Dynamic mechanical analyzer measures the temp. dependence modulus and stiffness. - Free mobility of polymer chains => lower storage modulus, so incorporating $CaCO_3$ raises it. PLA and nano-$CaCO_3$ also form structure together that may increase strength. - Improved loss modulus as well - Nano-$CaCO_3$ incorporated PLA is stiffer and responds better to temperature stress. - CO_2 emissions of the individual components of the bioplastic. **How does it answer the CQ?** - This analysis helps characterize the thermomechanical properties of PLA incorporated with nano-particle $CaCO_3$, suggesting applications towards packaging. **How does it impact the field?**

	The authors have proved that blending PLA with nano—CaCO3 improved thermomechanical properties, providing a viable solution to the issues with fossil plastics.
Research Question/Problem/ Need	Does PLA incorporated with bio-based nanoparticle CaCO3 exhibit improved thermomechanical properties compared to neat PLA?
Important Figures	 **Figure 3.** TGA thermogram curve of unfilled and nano-$CaCO_3$ reinforced polylactic acid bioplastic films. The curve from the thermal gravimetric analysis. Neat PLA begins to degrade around 200 degrees Celsius, while the nano-CaCO3 incorporated plastic is resilient until 350+ degrees Celsius.

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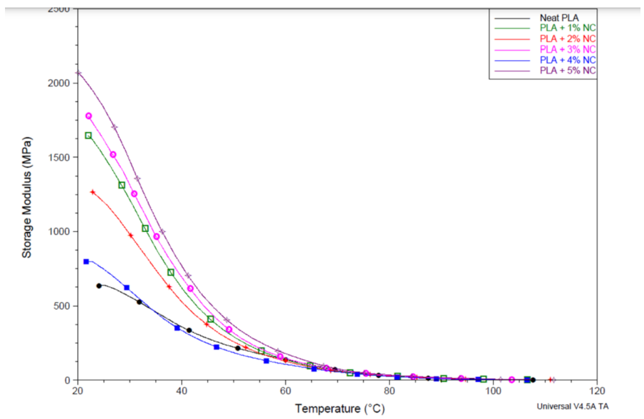

Figure 5. Storage modulus unfilled and nano-$CaCO_3$ reinforced polylactic acid bioplastic films.

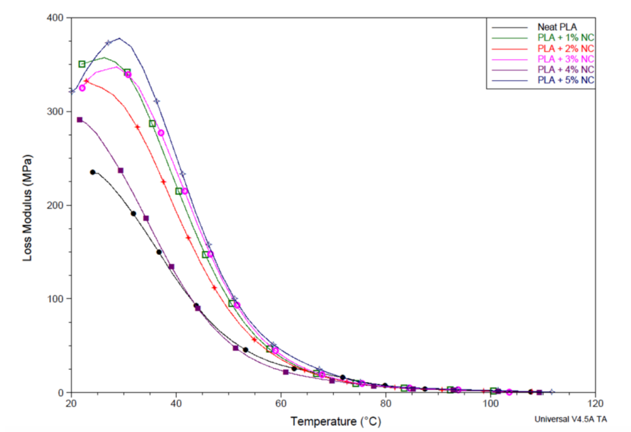

Figure 6. Loss modulus of unfilled and nano-$CaCO_3$ reinforced polylactic acid bioplastic films.

Nano-CaCO3 incorporated PLA has a higher storage modulus and a lower loss modulus. This means that the plastic is returning to its original shape under deformation rather than dissipating this energy as heat.
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<tr>
<td>VOCAB: (w/definition)</td>
<td>Polymer matrix – In a composite material that involves polymers, the matrix is the polymer backbone that forms a solid structure that holds fillers within
Fillers – particles added to polymers to improve their properties
Nanoparticles – 1 to 100 nm diameter particles</td>
</tr>
</table>

	Nanofiller = Fillers that are nanoparticles Thermogravimetric analysis – measuring mass as temperature changes Storage modulus, loss modulus = Young's modulus – the energy stored in the material when it is deformed by stress, and the energy lost by conversion to heat under the same conditions.
Cited references to follow up on	- López et al., 2015 for information on how/why nano-particles are used to reinforce bioplastics. - Nan et al., 2016, for why biomass is necessary to achieve these improved properties. - Samal et al., 2009, for more investigation into the properties of nano-$CaCO_3$ and how it affects polymers.
Follow up Questions	- Why do the particles used to reinforce bioplastics specifically have to be at the nanoscale? - Why is it necessary that the plastic incorporates nano-$CaCO_3$ from biomass, and not produced from any other method? - How biodegradable and toxic is the resultant plastic frm this research?

Article #10 Notes: 9/24/24 – Creation of a contractile biomaterial from a decellularized spinach leaf without ECM protein coating: An in vitro study

Article notes should be on separate sheets

Source Title	Creation of a contractile biomaterial from a decellularized spinach leaf without ECM protein coating: An in vitro study
Source citation (APA Format)	Robbins, E. R., Pins, G. D., Laflamme, M. A., & Gaudette, G. R. (2020). Creation of a contractile biomaterial from a decellularized spinach leaf without ECM protein coating: An in vitro study. *Journal of biomedical materials research. Part A, 108*(10), 2123–2132. https://doi.org/10.1002/jbm.a.36971
Original URL	https://doi.org/10.1002/jbm.a.36971
Source type	Journal Article
Keywords	Biomaterials, tissue engineering, regenerative medecine
#Tags	#Biomaterials, #biomedical, #tissue engineering
Summary of key points + notes (include methodology)	**Summary/Why is this important?** - Myocardial infarction is a dangerous condition that could lead to heart failure. hiPS-CMs can aid this, and decellularized spinach leaves provide a scaffold for it to happen. The researchers then needed to determine what they should coat the leaves with, and whether they need a fibronectin coating for the same result. - Researchers measured many metrics relating to cardiomyocyte health, including contractile strain, sarcomere length, and cell spreading, all of which they found to be statistically insignificantly different from coated leaves. **Notes** - **Motivation** - An infarcted heart with a tissue engineered patch would still need vasculature to receive nutrients.

	- A biomaterial with a vascular system within would easily solve this issue. - Past researchers used mammal tissue, these ones used spinach. - Fibromectin and other ECM proteins allow the cardiomyocytes to adhere to the surface, but they need to be obtained from donors. - Testing if ECM coating is necessary. - **Methods** - Spinach leaves were decellularized before the experiment, then water was removed. - Used 10 microg/ml of fibronectin coating. - The hiPS-CMs were created by genetically reprogramming adult somatic cells to behave like embryonic stem cells. - The cells were then differentiated into cardiomyocytes. - Placed onto both coated and non-coated spinach leaves. - Contractile function is defined by measuring strain in the left ventricle, which can be done with a microscope with a camera. - Measured maximum contractile strain. - Higher sarcomere length => higher maturity and contractile function, so used Immunofluorescence (IF) Imaging to measure Sarcomere length - Spread hiPS-CM onto the scaffolds, mature if their sarcomeres extended beyond the cell nucleus. - T-test for statistical significance. - **Results** - hiPS-CMs adhered with and without ECM coatings. - No statistically significant differences in contractile strain. - No statistically significant difference in sarcomere length. - No differences in cell spreading. **Significance** - The researchers have thus engineered a scaffold that is both plant-based and does not rely on impractical protein coatings, which could help diseased cardiac tissue recover.
Research Question/Problem/ Need	Do spinach biomaterial scaffolds used to restore contractile function to an infarcted heart require ECM coatings?
Important Figures	No statistically significant differences in contractile strain, no statistically significant difference in sarcomere length, and no

	differences in cell spreading. This tells you non-ECM coated leaves are just as effective for restoring contractile function. No pictures in the paper.
VOCAB: (w/definition)	Cardiomyocytes – Heart muscle cells which help it contract Pluripotent – a cell that's able to turn into multiple cell types hiPS-CMs - human induced pluripotent stem cell-derived cardiomyocytes ECM = extracellular matrix fibronectin – a protein found in the extracellular matrix of the heart Sarcomere – muscle tissue in the heart involved with contraction
Cited references to follow up on	- Modulevsky et al., 2007, for a description of an alternative to decellularized leaves, cellulose, for tissue engineering applications - Hansen et al., 2018, to find out what exactly makes a material attractive for cardiomyocytes to adhere to.
Follow up Questions	- What was the rational for ECM protein coatings in the first place? - How can this tissue-engineering solution be applied in vivo or to practical therapeutic application? - What advantages does fibronectin pose for a biomaterial in this application?

Patent #1 Notes: 10/4/24 – Nano engineered eggshell flexible biopolymer blend and methods of making biopolymer blend film and using such bioplastic blends for improved biodegradeable applications

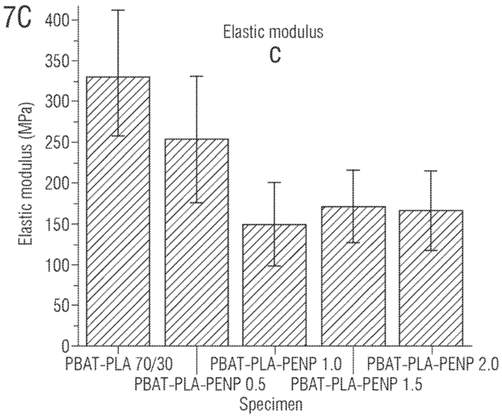
Article notes should be on separate sheets

Source Title	Nano engineered eggshell flexible biopolymer blend and methods of making biopolymer blend film and using such bioplastic blends for improved biodegradeable applications.
Source citation (APA Format)	Rangari, V., & Tiibomb, B. (2024, March 28). *Nano engineered eggshell flexible biopolymer blend and methods of making biopolymer blend film and using such bioplastic blends for improved biodegradeable applications.* (U.S. Patent No. 11613648). U.S. Patent and Trademark Office.
Original URL	No permanent URL
Source type	Patent
Keywords	Biopolymer, bioplastics, sustainability
#Tags	#PLA, #nanoparticles
Summary of key points + notes (include methodology)	**Summary/Why is this important?** - This patent provides a novel blend of PLA, PBAT, and eggshell nanoparticles to develop a new biodegradable and functional polymer. This can be used to encourage sustainability and reduce plastic pollution in the world. **Notes** - PLA is not ductile enough for many applications, extremely brittle. - Nano materials can help but no sufficient one exists. - The new biopolymer consists of PLA, PBAT, and PENP with the former two at a 70:30 ratio. - The PENP improves tensile strength, stiffness, and durability of the biopolymer. - Both the PBAT and PLA are sourced agriculturally.

	Preparation - Chicken eggshells dried and crushed using a mortar. - They used a "ball milling" technique to crush these chicken eggshells to somehow turn it into nanoparticles. - Carboxylic groups in the eggshells accord with the PLA and PBAT improving integrity of the polymer. - The PBAT and PLA are melt blended together, and the polymer film is created using an extrusion machine. **Methods** - Researchers performed a Raman microscopy analysis of the biopolymer. This provides information about the functional groups of the polymer. - X-Ray diffraction was performed to analyze the morphology of the blended polymers. This involves firing x-rays at the polymer to determine its chemical structure. - Transmission electron microscopy was performed to determine the size of the particles of the PENP. This is essentially shooting beams at a substance to try and image it at an extremely small scale. - A differential scanning calorimeter was necessary to study the thermal properties of the biopolymer. - Thermal gravimetric analysis (TGA) and tensile testing was also performed. **Results** - The PENP particles are the desired nanometer scale size and form a crystal-like structure. - The Raman analysis told the researchers that the different components of the blend did not interact much chemically, which is a good thing. - Thermal and mechanical analysis included in figures section.
Research Question/Problem/ Need	Which polymer blend of PLA, PBAT, and chicken eggshell nanoparticles have the most optimal thermal and mechanical properties?

Important Figures

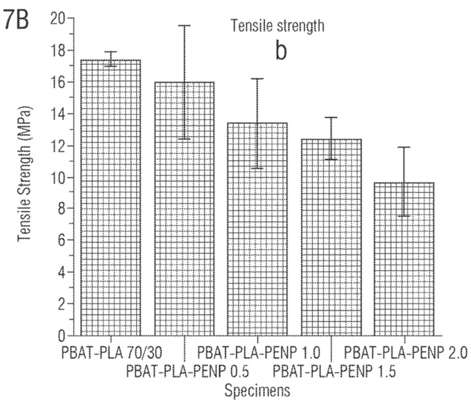
FIG. 7C



Tensile analysis of PBAT/PLA/PENP blend composites (elastic modulus)

Elastic modulus is the same as Young's modulus. A higher elastic modulus means a material is stiffer and will resist more deformation than otherwise. Thus, since the 70/30 blend of PBAT and PLA has the highest modulus, it is most likely the best mechanically. However, the 0.5 blend's modulus is still within one standard deviation of the 70/30 blend, making it inconclusive whether it really performed better.

FIG. 7B



Tensile analysis of PBAT/PLA/PENP blend composites (tensile strength)

70/30 most likely had the best tensile strength, but the test is still inconclusive due to the large error bars.

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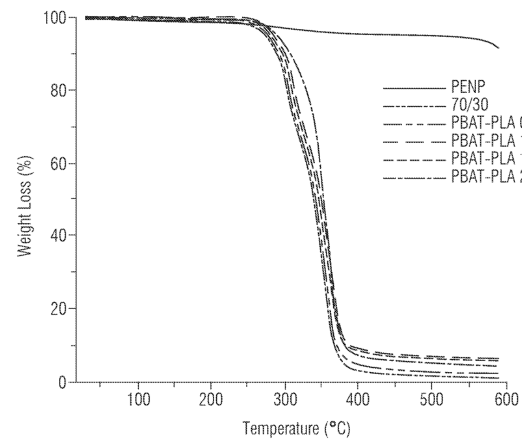
<tr><td></td><td>


Thermal degradation of PENP and PBAT/PLA/PENP blend composites

This is the TGA of the different polymer blends. It is clear from the graph that there is not much difference between the thermal properties of the blends. However, the 1.0 blend has a slight edge as the temperature exceeds 400 degrees Celsius.

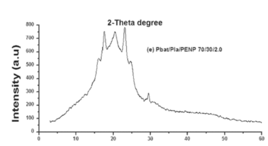


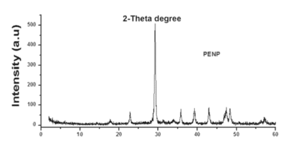
FIG. 3E: Xray diffraction pattern of Pbat/Pla/PENP 70/30/2.0


FIG. 3F: Xray diffraction pattern of PENP

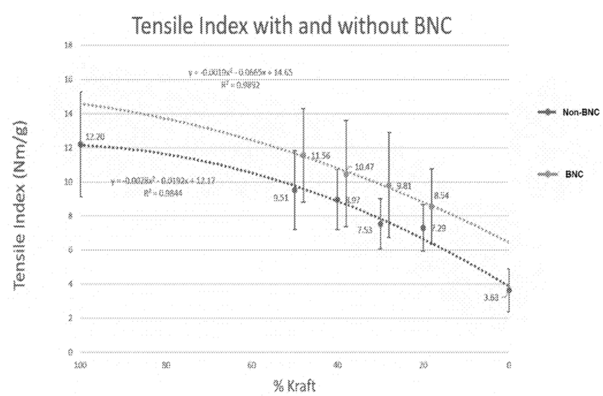
X-Ray diffraction pattern of PENP vs. the blend with 2.0 equivalences of PENP. Note the matching peaks in absorbance at 30 degrees on both graphs.
</td></tr>
<tr><td>VOCAB: (w/definition)</td><td>PBAT = polybutylene adipate terephthalate, a synthetic polymer
PENP = Proteinaceous eggshell nanoparticles</td></tr>
<tr><td>Cited references to follow up on</td><td>N/A, the patent does not cite any sources.</td></tr>
<tr><td>Follow up Questions</td><td>- What is the difference in the benefit of using a Raman microscopy analysis vs an FTIR to compare the chemical structures of a polymer?</td></tr>
</table>

	- What are the benefits and costs of the bioplastic PBAT on its own, without something to blend with? - What is the purpose and function of an extruding machine to create plastics? - What affects the margin of error in a tensile analysis?

Patent #2 Notes: 10/6/24 – Cellulosic fiber additive formed from Kombucha biofilms

Article notes should be on separate sheets

Source Title	Cellulosic fiber additive formed from Kombucha biofilms
Source citation (APA Format)	Moshasha, S., Grathwohl, C., & Mahoney, J. (2024, September 24). *Cellulosic fiber additive formed from Kombucha biofilms.* (U.S. Patent No. 12098508). U.S. Patent and Trademark Office.
Original URL	No permanent URL
Source type	Patent
Keywords	biomaterials, bio-based, sustainability
#Tags	#cellulose, #packaging, #biosynthesis
Summary of key points + notes (include methodology)	**Summary/Why It's important** - The paper provides a method in which Kombucha can be fermented using a colony of bacteria and yeast to produce nano-crystalline cellulose. This cellulose can be used to augment current paper products or replace them altogether. **Notes** - Cellulose manufacturing has existed for hundreds of years, but it is only recently that scientists could microfibrillate cellulose from plants. - While the production of nanocellulose is usually expensive industrially, the researchers have provided a cheap solution involving Kombucha fermentation. - Using this bacteria cellulose to add to wood products is a novel application that has not been tried yet. - Kombucha tea forms a biofilm when heated, called a SCOBY (Symbiotic colony of bacterial yeast). - Bacterial cellulose retain water extremely well and are more pure than other sources of cellulose. - This kombucha bacterial cellulose improves the mechanical properties of paper products when they are blended. - It forms complex web shaped formations with other polymers to improve their tensile strength and other properties.

	- The Kombucha cellulose can be used as an additive blended at a 1% composition with paper. - It can also be used to improve the properties of bioplastics such as PVA, PLA, etc., possibly even serving as a substitute for plasticizers. **Methods/Results** - Researchers measured the tensile strength of paper as fiber additives were mixed at different ratios. After performing a quadratic regression, the researchers determined that a higher amount of the cellulose produces a higher tensile strength. This cellulose originates from the kombucha SCOBY.
Research Question/Problem/ Need	How can bacterial nanocellulose be produced from Kombucha fermentation?
Important Figures	 FIG. 2B Adding bacterial nano cellulose to paper products generally improves its tensile index, regardless of a decreasing percentage of fiber. The difference relatively constant throughout, indicating that the cellulose additive always has a positive impact.
VOCAB: (w/definition)	Microfibrils/nanofibrils – small strands that make up cellulose. Nanocellulose – cellulose with its fibrils on the nano scale (2 – 100 nm) SCOBY – Symbiotic colony of bacterial yeast. Kombucha – An herb usually used to prepare tea.

Cited references to follow up on	- Azaredo et al., 2016, for more information about how nanocellulose can be applied to food packaging. - Yamanaka et al., 2011, for an application of nanocellulose to improving existing bioplastics.
Follow up Questions	- Why do the cellulose fibrils have to be specifically at the nano scale to improve the strength of paper products? - Can these additives be applied to plastic polymers rather than simply paper? - What are the costs associated with creating an environment conducive to a SCOBY forming? - How do cellulose additives affect other properties of paper – e.g., flammability?

Article #11 Notes: 10/13/24 – A molecular dynamics approach to modelling oxygen diffusion in PLA and PLA clay nanocomposites

Article notes should be on separate sheets

Source Title	A molecular dynamics approach to modelling oxygen diffusion in PLA and PLA clay nanocomposites
Source citation (APA Format)	Lightfoot, J. C., Castro-Dominguez, B., Buchard, A., & Parker, S. C. (2023, April 18). A molecular dynamics approach to modelling oxygen diffusion in PLA and PLA clay nanocomposites. *Material Advances, 2*(4), 2281-2291. https://doi.org/10.1039/D3MA00158J
Original URL	https://doi.org/10.1039/D3MA00158J
Source type	Journal Article
Keywords	Biopolymer, bioplastics, sustainability
#Tags	#PLA, #nanoparticles
Summary of key points + notes (include methodology)	**Summary/Why It's important** - Plastic pollution is harming the environment due to traditional plastics being non-biodegradable, and plastic packaging makes up 38% of plastic consumption. PLA is considered one of the most promising biodegradable alternatives to ordinary plastics, but it does not have ideal properties with respect to gas diffusion (barrier performance). Adding nanoparticle "fillers," especially made of clay, to improve these properties has been proven in real world tests, but not by mathematical models. The researchers used molecular dynamics and Monte-Carlo simulations to model the gas diffusion of a composite of clay and PLA. **Notes** - Barrier performance is an important property of PLA, since it can prevent the product packaged within from being spoiled or harmed. - Clay helps reduce gas diffusion as the gas particles must take harder pathways through the polymer to get through. Many

	clays such like mica, smectite, etc. have already been tried in a PLA composite. - While simple mathematical models already exist for predicting gas permeability in polymers, they do not work well in complex situations. Thus an MD simulation appealed as a way to pin down these complex chemical interactions. - Researchers used a force field called OPLS_2005 to model the interactions within PLA. - In the simulation, the system was compacted, then returned to ambient conditions. Then annealing was simulated on it. The clay that was added to the PLA was pyrophyllite. - Dihedral angles were "measured" in the simulation while the system was kept at constant temperature and pressure, to compare to real-world data later. - To simulate oxygen diffusion, the system was saturated with oxygen with randomly generated velocities, then diffusion was calculated as average squared displacement over 20 simulations of 200 ns - The energetic and structural properties of PLA were compared from the simulation to experimental data, and it was generally a good match. The amorphous density and distribution of dihedral angles were some of these properties. They thus proved the OPLS model worked to simulate PLA. - They modeled the composite PLA as well and checked the same dihedral angles. They were generally the same, telling us that the composite model worked adequately. - The density of the composite PLA in the model was very similar to that of the neat PLA, both averaging 1.19 g/cm^3. **Results** - Oxygen diffusion of neat PLA matched the experimental value of 1.37 * 10^(-8), within one standard deviation of it. - Oxygen diffusion was x lower in composite PLA. - Anisotropic diffusion was measured as well (important in composite system since diffusion might be directional due to large clay walls forming) and matched experimental values well. - Fractional free volume is 0.197 of original and 0.179 in composite – shows that composite is denser. - The researchers thus have shown their ability to simulate PLA composites with molecular dynamics.

Research Question/Problem/ Need

How does one create a molecular dynamics simulation that accurately characterizes oxygen diffusion in composite PLA with pyrophyllite nanoparticles.

Important Figures

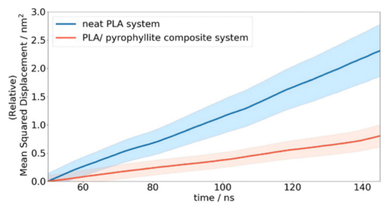


Fig. 7 Average oxygen MSD plots in a neat PLA and PLA/clay composite slab system. Coloured regions depict the standard error associated with the mean squared displacement across 20 duplicate simulations.

This diagram tells us that there is much more permeability of oxygen over time in neat PLA simulations relative to the ones with PLA nanocomposites, since the line for oxygen displacement for the neat PLA is consistently much higher.

Table 1 Structural and energetic parameters of crystalline PLA, obtained from DFT and MD calculation, and previously published experimental data

	DFT	MD	Experiment
$E_{\text{interfacial}}$/J m^{-2}	0.119	0.092	—
ρ_{crystal}/g cm^{-3}	1.314	1.274	1.29

Properties of the simulated neat PLA match those from real-world experiments and previous methods, telling us that the simulations are adequate.

VOCAB: (w/definition)

Barrier Performance – How well oxygen or water transmit through a surface/material.
Molecular dynamics (MD) – Simulation technique that tries to determine how atoms and molecules individually move.
Monte-Carlo simulation – Random simulation.
Delamination – breaking down by splitting into layers.
Interfacial – With a boundary of two types of matter
Density Functional Theory – a math modeling method that can determine the chemical interactions within materials.
Force field – jargon for molecular dynamics. A function that gives you potential energy of a molecule given its position.
Amorphous – non-crystalline, disordered structure
Fractional free volume – fraction of a material that is not occupied by its molecules

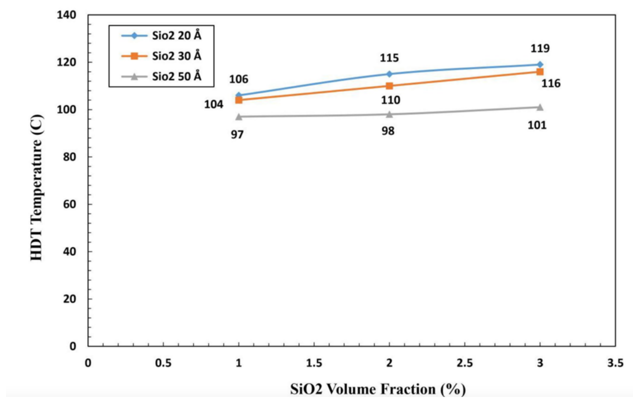
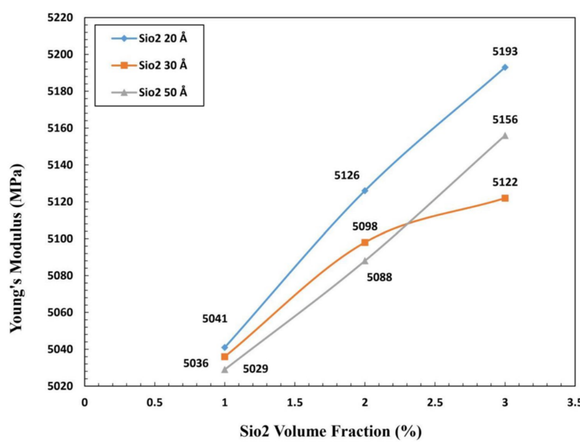
Cited references to follow up on	- Citations 6-10 can be useful to cite in the grant proposal - Castro-Aguirre et al., 2018, for information on how affinity between nanoparticles and PLA can be improved. - Singha et al., 2020, for general review of PLA and clay nanocomposites. - Morimune-Moriya et al., 2022, for more investigation to the factors that can affect clay's effectiveness in impoving PLA.
Follow up Questions	- What benefits does pyrophyllite pose over other types of nanoparticle clay? - How does clay disperse within PLA and how does that affect its properties? - How well do molecular dynamics simulations measure other properties of plastics, e. g. young's modulus, biodegradability?.

Article #12 Notes: 10/13/24 – Thermo-mechanical properties of silica-reinforced PLA nanocomposites using molecular dynamics: The effect of nanofiller radius

Article notes should be on separate sheets

Source Title	Thermo-mechanical properties of silica-reinforced PLA nanocomposites using molecular dynamics: The effect of nanofiller radius
Source citation (APA Format)	Nikzad, M. K., Aghadavoudi, F., & Ghasemi, F. A. (2024). Thermo-mechanical properties of silica-reinforced PLA nanocomposites using molecular dynamics: The effect of nanofiller radius. *J Polym Res, 31*(44). https://doi.org/10.1007/s10965-024-03873-0
Original URL	https://doi.org/10.1007/s10965-024-03873-0
	Journal Article
Keywords	Biopolymer, bioplastics, MD Simulation
#Tags	#PLA, #nanoparticles
Summary of key points + notes (include methodology)	**Summary/Why It's important** - .Researchers prepared a molecular dynamics simulation that measured the mechanical properties (Young's modulus), and thermal properties (Heat deflection temperature) of PLA composites with silicate nanoparticles. They focused specifically on the impact of atomic radius of the particles. They found the nanoparticles improved these properties and it matched experimental results. This can pave the way for a better bioplastic that could replace existing plastics to reduce pollution. **Notes** - Nanocomposites have less weight. - Silicate nanoparticles increase mechanical strength and decrease thermal degradation of PLA - Silica nanofillers were added at different atomic radii of 20 A, 30 A and 50 A with volume fractions of 1-3%

	- For molecular dynamics, one must first determine the initial position and velocity of each particle, as well as choosing a function to represent their potential energy, using Newton's motion equations to simulate the system over time - The force field used for the PLA is called DREIDING and the one used for silicate is called the Embedded Atomic Model (EAM). DREIDING involves 4 simple equations to describe the potential energy. - EAM is usually used for metals and metal alloy simulations. - To calculate Young's modulus they apply a small strain to the polymer and measure the resulting stress by an equation called virial stress - The resulting Young's modulus is calculated using Hooke's law - "Periodic boundary conditions" are used so that the simulation of a small part of the polymer can extend to actual cases - The temperature was 300K and the number of atoms, volume of the system, and temperature was all controlled with a 0.0001s step for the simulation - HDT was calculated by determining Young's modulus at different temperatures and finding where it drops heavily - Two steps for MD simulations: reaching equilibrium, and measuring properties. For equilibrium, energy and density both have to converge. **Results** - Young's modulus was extracted as 1.533 mPa for PLA which matches experimental values - Young's modulus increases with nanoparticle composition and is not affected by atomic radius - HDT increases with nanoparticle composition and decreases when atomic radius increases
Research Question/Problem/ Need	How does one create a molecular dynamics simulation that accurately characterizes mechanical and thermal properties in composite PLA with silicate nanoparticles?

Important Figures	 According to the graph, an increase in silica volume fraction leads to an increase in Heat Deflection Temperature as well. 

<table>
<tr><td></td><td>There's a similar stark increase for silica volume fraction vs. Young's modulus.
Table 2 The Young's modulus of PLA
<table><tr><th>Young's modulus (GPa)</th><th>Measurement method</th><th>Reference No.</th></tr><tr><td>1.41</td><td>Experimental tensile test</td><td>[29]</td></tr><tr><td>1.55</td><td>Experimental tensile test</td><td>[30]</td></tr><tr><td>1.58</td><td>Experimental tensile test</td><td>[31]</td></tr><tr><td>1.6</td><td>Experimental tensile test</td><td>[32]</td></tr><tr><td>1.7</td><td>Experimental tensile test</td><td>[33]</td></tr><tr><td>1.533</td><td>Simulation</td><td>Current study</td></tr></table>
MD simulation output matches experimental data pretty well.</td></tr>
<tr><td>VOCAB: (w/definition)</td><td>HDT - heat deflection temperature – the temperature at which a polymer deforms at a given load
Force field – Mathematical function that describes the potential energy of a particle, used to model interactions
Van der waals force – weak intermolecular forces that depend on their distance
Periodic boundary conditions – boundary conditions that allow you to approximate a large system using a small part of it</td></tr>
<tr><td>Cited references to follow up on</td><td>- . Jeon et al., 2022 for review on molecular dynamics simulations for nanocomposites.
- Daneshpayeh et al., 2021, for what factors of the silicate can affect mechanical properties.
- https://doi.org/10.1177/0095244324127078 by the same author – contains an experimental analysis that corresponds to this MD analysis.</td></tr>
<tr><td>Follow up Questions</td><td>- What software is the best to use for MD analysis of polymers?
- Why doesn't particle size have a large effect on the thermal properties of the PLA?
- How does one determine what force field to use for a certain part of the simulation?</td></tr>
</table>

Article #13 Notes: 10/20/24 – Research and applications of nanoclays: A review

Article notes should be on separate sheets

Source Title	Research and applications of nanoclays: A review
Source citation (APA Format)	Uddin, M. N., Hossain, M. T., Mahmud, N., Alam, S., Jobaer, M., Mahedi, S. I., & Ali, A. (2024). Research and applications of nanoclays: A review. *SPE Polymers, 5*(4), 507–535. https://doi.org/10.1002/pls2.10146
Original URL	https://doi.org/10.1002/pls2.10146
	Review Article
Keywords	Review, nanoclay, nanoparticles
#Tags	#review, #nanoparticles
Summary of key points + notes (include methodology)	**Summary/Why It's important** - .Nanoclays have shown applications for creating composite polymers, specifically in food packaging. Its other applications have led me to this review article on them and what types of nanoclays exist. The article also explains challenges with current nanoclay research. **Notes** - Nanoclays are low cost and have a low impact on the environment. - They form layered crystallites inside materials, in octahedral or tetrahedral shapes. - Adding nanoclays to materials improve "stiffness, strength, toughness, and thermal stability." - It has applications to electronics and to biomedical applications with controlled drug release. - Synthesizing nanoclays is a complicated process, which can involve either intercalation or exfoliation. Intercalation means inserting organic molecules between layers of the clay, which exfoliates it and increases the surface area. - Keeping nanoclays evenly distributed within a polymer leads to some difficulties since clay agglomerates easily - There are 3 main types of nanoclay

	○ Cationic nanoclays include ones like smectite and mica. ○ This happens when Mg replaces Al or Al replaces Si within the sheets, meaning there's a charge imbalance that cations from surrounding areas come in to solve, leading to swelling. ○ This makes it effective for polymer composites where better dispersion is needed ○ Examples: Montmorillonite, hectorite ○ Anionic nanoclays occur when there are trivalent cations within, making it effective in ion exchange ○ Neutral nanoclays contain no or low charge and have two tetrahedral sheets sandwiched with an octahedron sheet ○ They do not swell much or exchange ions, meaning they are effective when the material must be inert and stable, like in composites ○ Examples: Kaolinite - It has applications to aerospace, construction, automobiles, and biomedical fields, for which I won't go much in depth - Nanoclays are effective at shielding food and other products for packaging purposes - It improves mechanical, barrier, and thermal properties of plastic films - There are some challenges with adoption of nanoclays ○ It is necessary to study the properties and structure of nanoclays further. ○ Also the toxicity and impact on human health must be investigated. Synthesizing them is also difficult and unsafe.
Research Question/Problem/ Need	What are the benefits and applications of nanoclays?
Important Figures	

TABLE 1. Comparative analysis of all clay types with their advantages and disadvantages.

Name of nanoclay	Types	Key properties	Advantages	Disadvantages	Ref.
Montmorillonite	Cationic nanoclay	High cation exchange capacity Layered silicate structure Swellable in water	High surface area Good adsorption properties Enhances mechanical strength in composites	Requires surface modification for compatibility with non-polar matrices	[40]
Kaolinite	Neutral nanoclay	Low cation exchange capacity Layered silicate structure Non-swelling	Chemically inert Abundant and low cost	Limited intercalation capacity-Lower surface area compared to other clays	[82]
Hectorite	Cationic nanoclay	High cation exchange capacity	High viscosity in suspensions Good thermal	Expensive Limited availability	[41]

This is an incomplete figure containing the benefits of each clay type. The full figure is in the paper. The idea is that some nanoclays have advantages in different areas than others – montmorillonite enhances mechanical strength while kaolinite enhances thermal stability.

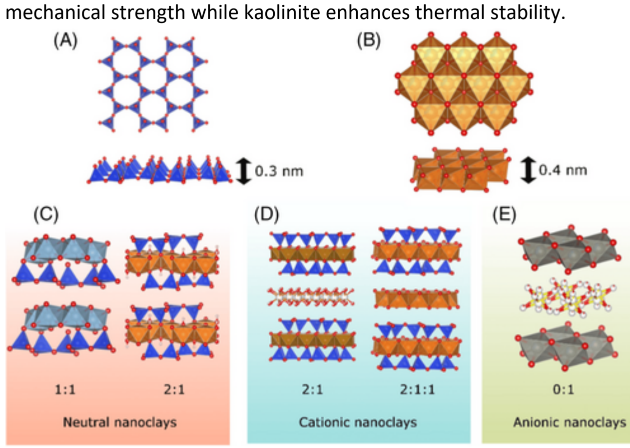


Figure explaining the structure of nanoclays in polymers as layers of tetrahedral and octahedral sheets.

VOCAB: (w/definition)	Aspect ratio – surface to volume ratio of a nanoparticle

	Agglomerate = accumulate Swelling = increasing volume due to solvent molecules
Cited references to follow up on	- Ray & Okamoto, 2003 – cited for information on solution intercalation of nanoclay, which is what I need to do.
Follow up Questions	- What conditions are needed for nanoclay to be evenly dispersed within a polymer matrix when combined in a solution? - How does combing two types of nanoclay affect the morphology and properties of the composite? - What causes the clays to result in very specific properties?

Article #14 Notes: 11/5/24 – Hybrid Pu/Synthetic Talc/Organic Clay Ternary Nanocomposites: Thermal, Mechanical and Morphological Properties

Article notes should be on separate sheets

Source Title	Hybrid Pu/Synthetic Talc/Organic Clay Ternary Nanocomposites: Thermal, Mechanical and Morphological Properties
Source citation (APA Format)	Dias, G., Prado, M., Ligabue, R., Poirier, M., Le Roux, C., Micoud, P., Martin, F., & Einloft, S. (2018). Hybrid Pu/synthetic talc/organic clay ternary nanocomposites: Thermal, mechanical, and morphological properties. *Polymers and Polymer Composites, 26,* 127-140. https://doi.org/10.1177/096739111802600201
Original URL	https://doi.org/10.1177/096739111802600201
	Journal Article
Keywords	Polyurethane, synthetic talc, ternary nanocomposites, organic clay, mechanical properties
#Tags	#composite, #nanoparticles
Summary of key points + notes (include methodology)	**Summary/Why It's important** - .Nanoclays mixed with polyurethane (PU) tend to improve its mechanical and thermal properties - Researchers added synthetic talc (SSMMP) and organically modified commercial clays (SPR) at modified weights - Test showed good dispersion of these clays within the matrix - Results showed improved Young's Modulus to regular PU. - This shows the success of ternary composites and this specific blend. **Notes** - Polyutherane is a plastic that is easily adaptable by adding inorganic particles to the matrix - Clays have high aspect ratios, making them important for improving mechanical properties - However, this requires on good dispersion within the polymer matrix

	- The fillers can be intercalated up to exfoliated - Synthetic talc is easily manufactured and the particle size range can be easily modulated - An ultrasound bath was used to disperse the fillers with metyl ethyl ketone as a solvent - Mechanical stirring was performed with a catalyst - Films were produced by casting and dried - **Tests** - X-ray diffraction, transmission electron microscopy, and FTIR were performed along with mechanical and thermal tests - **Results** - XRD showed many low intensity peaks showing well dispersion of talc - Crystal sizes were smaller than those of natural talc - The peaks of the individual fillers were reduced compared to the secondary composites - TEM showed well-dispersion, morphology is possibly exfoliated - FTIR showed the expected peaks, but a new one relating to Si-O-Si bonds stretching showing well dispersion - Thermal analysis showed degradation at a higher temperature - Young's modulus improved, showing interfacial interactions between the polymer and filler - Conclusion: good dispersion and improved properties
Research Question/Problem/ Need	How do synthetic talc and organically modified commercial clays disperse within polyutherane and affect its properties?

Important Figures

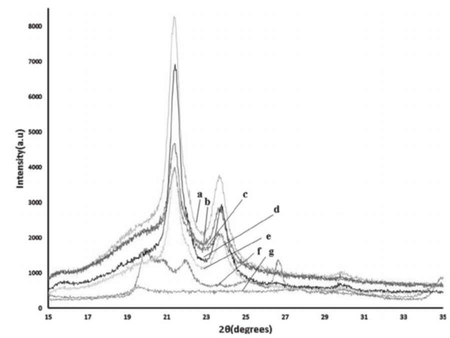


Figure 1. X-ray diffractogram patterns (a) PU, (b) PU/SSMMP 7 h+SPR 3% 25:75, (c) PU/SSMMP 7 h+SPR 3% 75:25, (d) PU/SPR 3%, (e) PU/SSMMP 7 h 3%, (f) SPR clay and (g) SSMMP 7 h

F and G are the X Ray Diffraction curves for the clays. They are relatively stable and low, showing well dispersion of the clay.

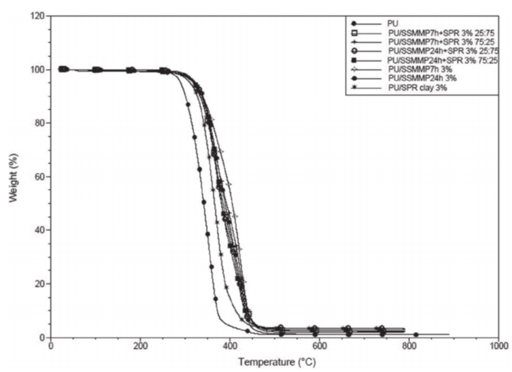
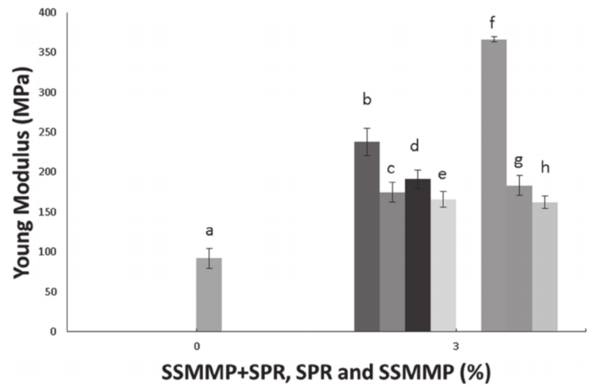


Figure 5. TGA curves for the pristine PU and the hybrid nanocomposites

Thermal gravimetric analysis, where the composites perform better than pure PU in terms of degradation when temperature increases.

	 **Figure 8.** Young's modulus values for hybrid nanocomposites and pristine PU (a) PU Pure; (b) PU SSMMP 7 3% 25:75; (c) PU SSMMP 7 h+SPR 3% 75:25; (d) PU SSMMP 24 h+SPR 3% 25:75, (e) PUSSMMP 24 h+SP 75:25, (f) PU/SPR clay 3%, (g) PU/SSMMP 7 h 3% and PU/SSMMP 24 h 3% The composites show improvement in Young's Modulus over pure PU. However, it is not as much of an improvement as PU + SPR 3%.
VOCAB: (w/definition)	Ternary composite – a composite where 2 different substances are added to the polymer matrix Polyutherane – a plastic that is easily adaptable by adding inorganic particles to the matrix Intercalated – the filler is inserted between the layers of the polymer Exfoliated – the filler is well-dispersed and creates its own layers within the polymer Transmission electron microscopy – using electrons to create an image
Cited references to follow up on	- Song et al., 2003 - Jin et al., 2010 - Osmal et al., 2014 - These are all papers on other ternary composites. It would be useful to read these papers to try and understand how these behave.
Follow up Questions	- Can simpler techniques be used for good dispersion of fillers within plastics? - Are ternary composites inherently better or worse than simpler ones?

	- How do the different clays interact together within the matrix to create improved properties?

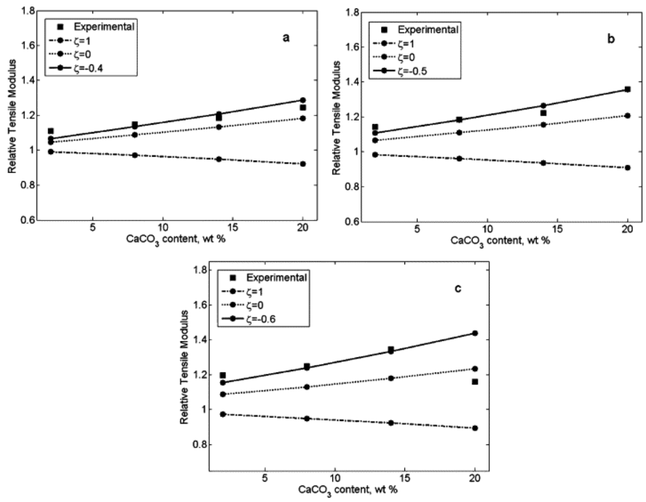
Article #15 Notes:- 11/10/24 – Modeling of interfacial bonding between two nanofillers (montmorillonite and CaCO3) and a polymer matrix (PP) in a ternary polymer nanocomposite

Article notes should be on separate sheets

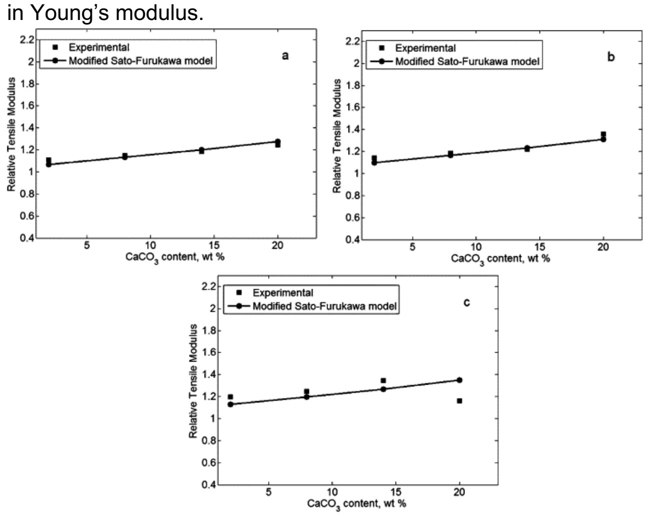
Source Title	Research and applications of nanoclays: A review
Source citation (APA Format)	Zare, Y., & Garmabi, H. (2014). Modeling of interfacial bonding between two nanofillers (montmorillonite and $CaCO_3$) and a polymer matrix (PP) in a ternary polymer nanocomposite. *Applied Surface Science, 321*, 219–225. https://doi.org/10.1016/j.apsusc.2014.09.156
Original URL	https://doi.org/10.1016/j.apsusc.2014.09.156
	Journal Article
Keywords	Ternary polymer nanocomposites, Adhesion at the interface, Mechanical properties.
#Tags	#composite, #nanoparticles
Summary of key points + notes (include methodology)	**Summary/Why It's important** - .The researchers attempted to create a simplified model to determine how two nanofillers interact within a polymer composite of PP (polypropylene) They then measured these compared to experimental results, and found a reasonably large interfacial adhesion between the two fillers. This information can be useful to further research on ternary nanocomposites of polymers. **Notes** - Nanofillers cause high stiffness and low flammability. - This is due to high surface area - Yield strength was considered the most important mechanical property

	- The materials were mixed using melt mixing with a screw extruder. Injection molding was then performed, then a tensile test. - 6% of montmorillonite and 14% of $CaCO_3$ led to the highest yield strength - X Ray diffraction was also performed, which showed well dispersion - A formula was used to estimate the yield strength of the composite based on the densities of the constituents. $$\sigma_R = \exp(-k\phi)$$ - σR is related to yield strength while phi is the nanofiller volume fraction. Thus a higher k value leads to a lower yield strength value and thus signals worse interfacial adhesion. - The results showed k was near 0 - Other models showed similar results - This is due to cation exchange reactions that make the hydrophobic polymer compatible with the nanofiller - The interactions are mostly van der Waals and the largest interactions are between the Hydrogen atoms on the polymer - There exists a model by Sato and Furukawa that predicts Young's Modulus using adhesion as a parameter - The researchers then improved on this model by removing the adhesion parameter by setting it to 0 for ternary nanocomposites by assuming good adhesion. This allows a simple prediction of Young's Modulus. - The researchers then tried fitting linear and quadratic models to weight % and yield strength.
Research Question/Problem/ Need	How does interfacial adhesion affect the strength of montmorillonite and $CaCO_3$ ternary nanocomposites?

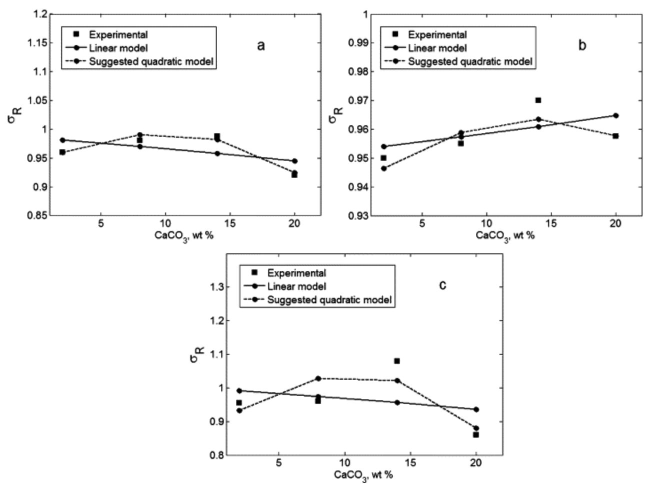
Important Figures



Using the Sato- Furukawa model, these are predicted Young's modulus based on weight % of CaCO3, assuming different values of interfacial adhesion. The results showed that experimental values were very close to the zeta=0 line, and also that increasing the calcium carbonate content led to an increase in Young's modulus.



This is the same result, except using the simplified model instead of Sato-Furukawa's. This removes the interfacial adhesion

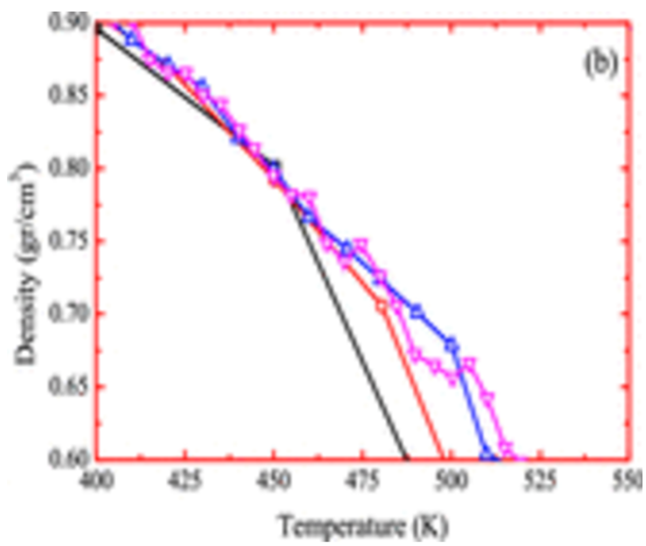
	parameter, and the results are very similar to experimental values.  Models of yield strength vs Calcium carbonate content, linear and quadratic fits. The quadratic model was the closest to experimental values.
VOCAB: (w/definition)	Polypropylene – A plastic used in many applications including packaging Screw extruder – A machine that turns a melting plastic into a continuous form Melt mixing – Mixing polymers in a molten state
Cited references to follow up on	- Sato & Furukawa, 1963 for an explanation of the original model for polymer composites
Follow up Questions	- Is it guaranteed that ternary nanocomposites will have strong interfacial adhesion? - What is the explanation behind the original Sato-Furukawa model? - Why do the ternary composites perform better than individual CaCO3 or clay composites?

Article #16 Notes:- 11/29/24 – Nanoparticle Shape Influence over Poly(lactic acid) Barrier Properties by Molecular Dynamics Simulations

Article notes should be on separate sheets

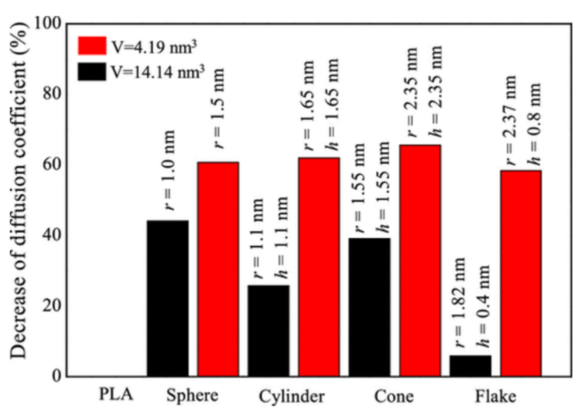
Source Title	Nanoparticle Shape Influence over Poly(lactic acid) Barrier Properties by Molecular Dynamics Simulations
Source citation (APA Format)	Prada, A., González, R. I., Camarada, M. B., Allende, S., Torres, A., Sepúlveda, J., Rojas-Nunez, J., & Baltazar, S. E. (2022). Nanoparticle shape influence over poly(lactic acid) barrier properties by molecular dynamics simulations. *ACS Omega, 7*(3), 2583–2590. https://doi.org/10.1021/acsomega.1c04589
Original URL	https://doi.org/10.1021/acsomega.1c04589
	Journal Article
Keywords	Nanoparticles, Poly(lactic acid), Barrier properties, Molecular dynamics simulations
#Tags	#composite, #nanoparticles, #MD
Summary of key points + notes (include methodology)	**Summary/Why It's important** - Molecular dynamics simulations were used to predict oxygen permeability of PLA nanocomposites. They attempted to figure out the impact of particle shape on the barrier properties, and found that the sphere is the best possible shape. This has applications to develop new sustainable materials and reduce the impacts of climate change. **Notes** - PLA's barrier properties need improvement for wider adoption - Nanoparticles have high impact due to high surface area - Previous research has not studied the impact of nanoparticle shape on performance - O2 permeability was tested using MD simulations - The DREIDING forcefield was used to generate the box while the CHARMM forcefield was used to create the simulations

	- MD simulations were performed using the LAMMPS software - PLA had 32 chains with 50 monomers each - The initial PLA had density and glass transition temperature measured - Density was compared at different temperatures and a linear correlation was found - Nanoparticles were tested as sphere, cylinder, cone, and flakes - Barrier properties were measured by adding 15% mass of oxygen to the system and measuring their displacements - **Results** - Neat PLA simulations values are relatively similar to experimental values - For nanoparticles with larger volumes, shape had a larger effect - Eventually the nanoparticle volume gets so large that it changes the characteristics of the original PLA - Spheres lead to the greatest reduction in oxygen diffusion, while narrower cylinders perform better than wide ones - For sphere and cone nanoparticles, there are surrounding regions that experience less oxygen displacement – this means these particles capture the oxygen molecules and reduce permeability on a macro scale - Oxygen interacts mostly with the hydrogens on the PLA molecules - Interaction of oxygen with other oxygen molecules also improves the retention - **Discussion** - Adding these nanoparticles might not be the optimal consideration due to a decrease in biodegradability when too much is added - When nanoparticles are agglomerated the opposite effect occurs.
Research Question/Problem/ Need	How does the particle size of nanofillers affect the barrier properties of PLA?
Important Figures	

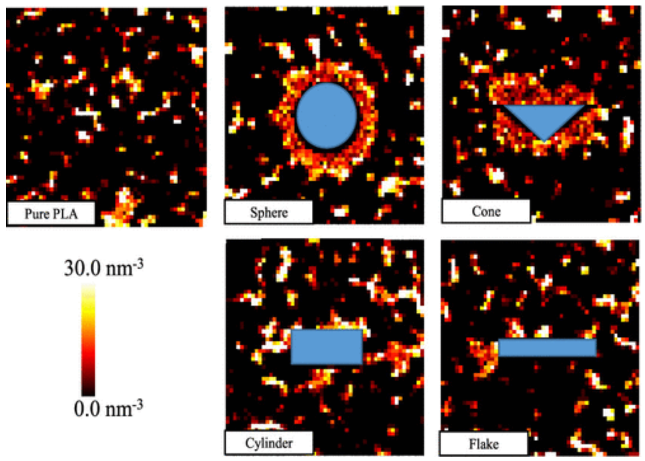


Density vs. Temperature shows a linear correlation across all the simulations. This shows that the simulation is reasonable and delivering realistic results.

Figure 3



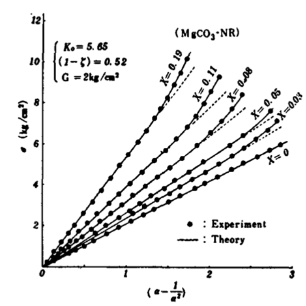
Sphere and cone nanoparticles lead to a greater reduction in oxygen diffusion than any other types. This is due to the agglomeration of oxygen molecules around those nanoparticles.

	 Oxygen occupation at different locations around the nanoparticle, over the last 1.5 ns of the simulation. Here the sphere and cones have surrounding regions with higher oxygen occupation – this shows that they capture the oxygen, allowing it to agglomerate and preventing permeation.
VOCAB: (w/definition)	Self-diffusion coefficient – how much particles move within a substance under equilibrium conditions NPT ensemble – N particles, pressure, temperature. A term for MD simulations where those three parameters are kept constant. NVT corresponds for volume instead of pressure.
Cited references to follow up on	- Petersson & Oksman, 2006, for an application of the same concept to clay - Alexandre & Dubois, 2000, for research offering an overview of silicate nanoparticles.
Follow up Questions	- Does the shape of nanoparticles have the same effect regardless of the substance that makes them up? - What shapes do clay nanoparticles form and what effect does that have? - Does size have an effect like shape does, and if so, what?

Article #17 Notes:- 12/7/24 – A Molecular Theory of Filler Reinforcement Based upon the Conception of Internal Deformation

Article notes should be on separate sheets

Source Title	A Molecular Theory of Filler Reinforcement Based upon the Conception of Internal Deformation
Source citation (APA Format)	Sato, Y., & Furukawa, J. (1963). A Molecular Theory of Filler Reinforcement Based upon the Conception of Internal Deformation (A Rough Approximation of the Internal Deformation). *Rubber Chemistry and Technology, 36*(4), 1081–1106. https://doi.org/10.5254/1.3539632
Original URL	https://doi.org/10.5254/1.3539632
	Journal Article
Keywords	Filler reinforcement, Polymer composites, Mechanical Properties
#Tags	#composite, #nanoparticles
Summary of key points + notes (include methodology)	**Summary/Why It's important** - Researchers have developed a model of mechanical properties of elastomers with fillers based on the effects on volume, surface, and cavitation. This allows a novel and useful characterization of the mechanisms of filler reinforcement. **Notes** - When the paper was written, there was no standardized or usable method of mechanical analysis for these materials. Also, modeling adhesion between filler and medium is complex. - Unknown how dispersion affects properties, so uniform dispersion was assumed for the paper - With this assumption, you arrive at the notion that the particles form a cubic lattice, and there exists a spherical domain (which they call a D-sphere) around each particle with the same radius

	- From this, the researchers determined that the volume fraction of the filler would thus be the cube of the ratio of particle radius to D-sphere radius - Adhesion is modeled as a mixture of two ideal states – perfect adhesion and perfect non adhesion (meaning a cavity) - To minimize the free energy of the system, its cavities must be ellipsoids - They determined an expression for the energy of deformation, which must be minimized - Tension of the system involves volume concentration, surface concentration (at the interface between the nanoparticle and the medium) and cavitation, determined by the volume and size of cavities. - Young's modulus can be determined by differentiating tension with respect to strain. However, it can increase when there is swelling. - The researchers thus came up with an expression that can estimate Young's modulus based on a coefficient of dispersion and volume fraction.
Research Question/Problem/ Need	How do fillers affect the mechanical properties of elastomers, and how can this be modeled?
Important Figures	 FIG. 6.—An example for relation of tension versus elongation in filled rubber vulcanizates[5]. Theoretical curves are calculated from Equation (28′). The theory estimates the stress and strain of rubber well in vulcanized rubber.

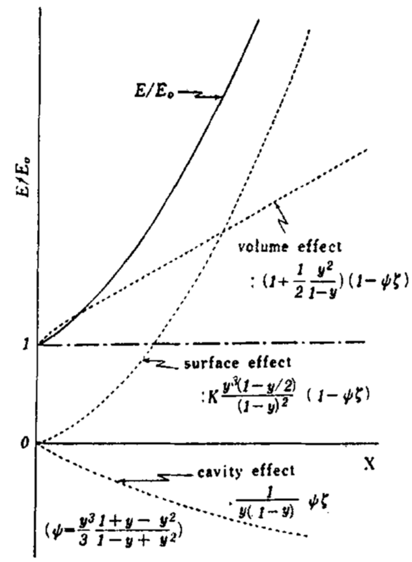


Fig. 7.—Three effects and reinforcing tendency in Young's modulus.

Influences of the 3 effects of composites on Young's modulus. Volume and surface effects increase it while cavities decrease it, which intuitively makes sense.

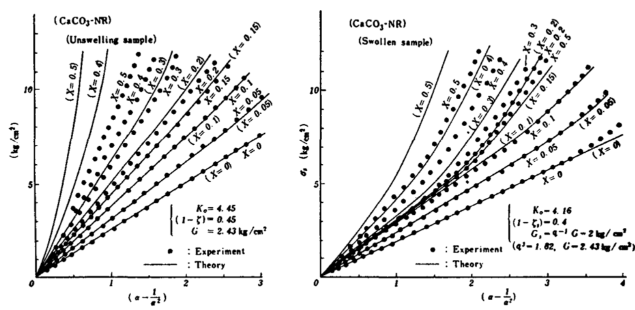


Fig. 11.—Comparison between tension σ and swelling tension σ_s. Theoretical curves are calculated from Equations (28′) and (37), respectively.

In swollen samples, Young's modulus is not constant. The model is able to adapt to this fact as seen by the fact that it matches experimental data.

VOCAB: (w/definition)	Cavitation – formation of cavities filled with vapor/voids due to deformation Internal deformation – deformation at a molecular level regardless of external changes
Cited references to follow up on	- There are no references in the paper.
Follow up Questions	- How do cavities form near nanoparticles? - How does the composition of the nanoparticles affect the adhesive properties? - Are there practical implications or applications of this theory in designing new composites?

Article #18 Notes:- 12/16/24 – New ternary PLA/organoclay-hydrogel nanocomposites: Design, preparation and study on thermal, combustion and mechanical properties

Article notes should be on separate sheets

Source Title	New ternary PLA/organoclay-hydrogel nanocomposites: Design, preparation and study on thermal, combustion and mechanical properties
Source citation (APA Format)	Shabanian, M., Hajibeygi, M., Hedayati, K., Khaleghi, M., & Khonakdar, H. A. (2016). New ternary PLA/organoclay-hydrogel nanocomposites: Design, preparation and study on thermal, combustion and mechanical properties. *Materials & Design, 110*, 811–820. https://doi.org/10.1016/j.matdes.2016.08.059
Original URL	https://doi.org/10.1016/j.matdes.2016.08.059
	Journal Article
Keywords	Nanocomposite; Thermal properties; Hydrogel; Organoclay; Synergic effect
#Tags	#composite, #pla, #nanoparticles
Summary of key points + notes (include methodology)	**Summary/Why It's important** - A new type of PLA-based nanocomposite was created using a hydrogel and an organoclay, with improvements in strength, heat resistance, and combustion safety at the same time - It addresses the common weaknesses of PLA like low durability and high flammability, making it more suitable for demanding applications. **Notes** - PLA has issues with respect to its low thermal stability, high combustibility, and melt dripping limit - Organoclays lead to good dispersion and compatibility of hydrophilic hydrogels in hydrophobic PLA

	- The new nanocomposite uses this synergistic effect to improve the mechanical properties, combustion resistance, and thermal stability of PLA - Organoclay was made from a surface modification of montmorillonite - Solvent casting was performed to create the samples with sonication to improve dispersion - FTIR spectra were created and X-ray diffraction was performed - Thermogravimetric analysis and tensile tests were done, as is usual - **Results** - FTIR spectra showed remnants of the reaction performed to create the organoclay. - Hydrogel's characterization showed that the coupling reaction used to form it was successful. - Strong hydrogen bonds were observed between the hydrogel and PLA - X-ray diffraction showed successful intercalation - The composites displayed improved thermal stability - Microscale combustion calorimetry was used to measure combustion, and the composites had lowered values for this. - The hydrogel had no improvement in Young's modulus on its own, however it worked synergistically with the organic clay to improve Young's modulus - Thermal, combustion, and mechanical properties all improved, which is surprising to all happen at the same time
Research Question/Problem/ Need	How do hydrogels and organoclays work synergistically to improve the properties of PLA?

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<td>Important Figures</td>
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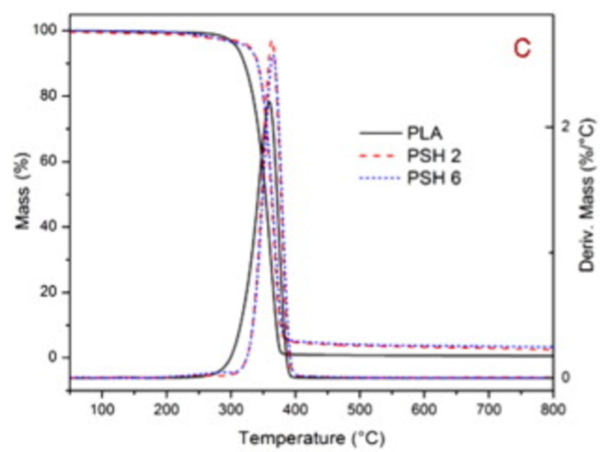
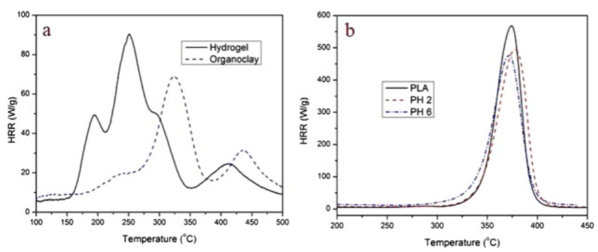


This measures thermal degradation as temperature increases. For the composites, the curve is to the right of neat PLA, showing later degradation.



Combustion data for hydrogel and organoclay, and the PLA composites. The composites release much less heat from combustion than neat PLA.
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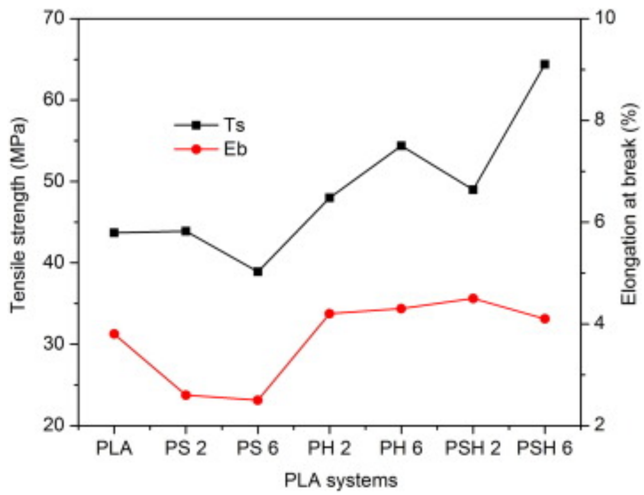
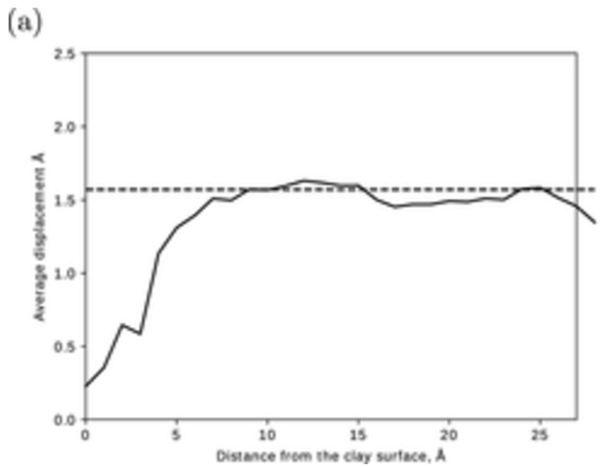
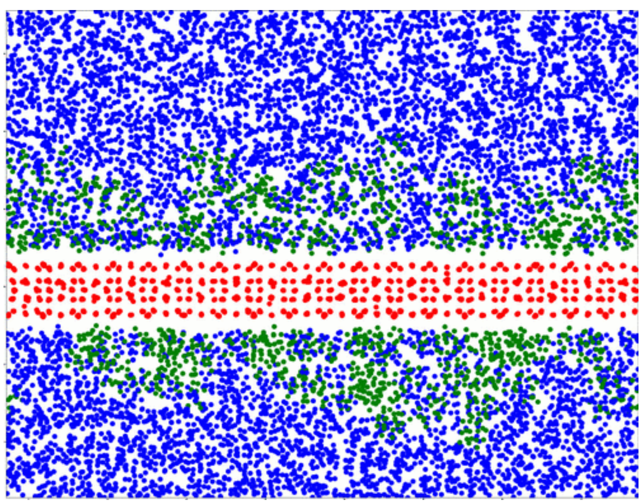
	 Tensile strength and elongation at break are both increased by the composite PLA systems.
VOCAB: (w/definition)	Organoclay – Modified organophilic clay made through cation exchange Microscale combustion calorimetry – Measuring the rate of heat flow from combustion
Cited references to follow up on	- Lim et al., 2008, for a review on processing PLA - Ray et al., 2002, for general information on PLA-silicate composites
Follow up Questions	- Why do nanoclays improve flame retardancy? - Is sonication necessary for dispersion of nanoparticles in PLA solutions? - How do hydrogels affect polymers in general?

Article #19 Notes:- 12/17/24 – Molecular Dynamics Study of Ternary Montmorillonite–MT2EtOH–Polyamide-6 Nanocomposite

Article notes should be on separate sheets

Source Title	Molecular Dynamics Study of Ternary Montmorillonite–MT2EtOH–Polyamide-6 Nanocomposite: Structural, Dynamical, and Mechanical Properties of the Interfacial Region
Source citation (APA Format)	Skomorokhov, A. S., Knizhnik, A. A., & Potapkin, B. V. (2019). Molecular Dynamics Study of Ternary Montmorillonite–MT2EtOH–Polyamide-6 Nanocomposite: Structural, Dynamical, and Mechanical Properties of the Interfacial Region. *The Journal of Physical Chemistry B, 123*(12), 2710–2718. https://doi.org/10.1021/acs.jpcb.8b10982
Original URL	https://doi.org/10.1016/j.matdes.2016.08.059
	Journal Article
Keywords	Ternary polymer nanocomposites, Molecular dynamics, Mechanical properties.
#Tags	#composite, #nanoparticles, #MD
Summary of key points + notes (include methodology)	**Summary/Why It's important** - Researchers developed a new plastic based on polyamide-6 and montmorillonite and MT2EtOH using MD simulations. - They characterized the structure and calculated Young's Modulus of the composite - Regions near the surface of the clay had the highest Young's modulus. - They were able to model the thickness of the interfacial region was well by predicting how the nanoparticles affect it. - This can lead to development of new sustainable plastics. **Notes** - Montmorillonite usually does not achieve optimal exfoliation when added to polymers

	- Some sort of treatment is required, for example with polar organic molecules, like MT2EtOH - Experiments cannot determine microscopic properties of these polymers, making MD simulations necessary - The energy of the interactions between the Montmorillonite, organic clay, and polymer were all measured - MMT was formed by making substitutions of atoms in pyrophyllite with cations - The systems had to be relaxed at thermal equilibrium before the measurements could begin - The LAMMPS software was used to perform the simulations - Young's modulus was measured by applying stress and measuring the strain of the system - Interlayer space and density generally matched experimental values in the simulations - There was a profound difference in results regarding whether the organic modification was placed uniformly or near the nanoparticles. However, this difference eventually relaxed to the same structure. - They determined that the properties of the small slice of the polymer reflect the overall results - Atoms near the clay were restricted in their movements, which is beneficial - Interfacial region was two times as hard as normal PLA
Research Question/Problem/ Need	How do MT2EtOH and montmorillonite affect the properties of polyamide-6?

Important Figures	 Being near the clay nanoparticles have a negative effect on atomic mobility. This improves the strength of the composite.  A figure showing a snapshot of the simulation, where red is montmorillonite, blue is the polymer, and green is a modifier. This shows that montmorillonite forms uniform layers with the polymer.
VOCAB: (w/definition)	Polyamide – a type of thermoplastic with unusually good mechanical properties

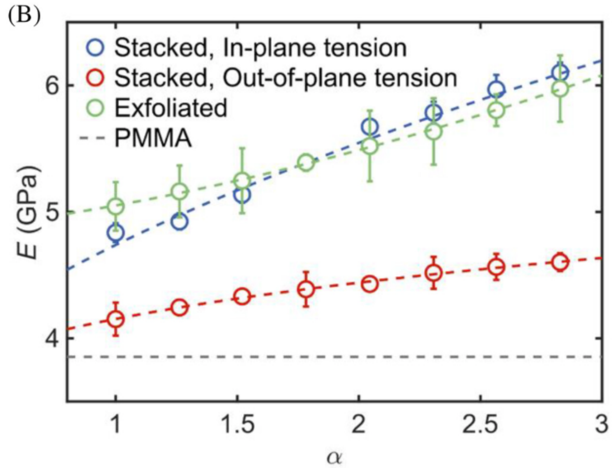
	MT2EtOH – a specific polar organic molecule.
Cited references to follow up on	- Leszczyńska et al., 2007, for more info on MMT composites
Follow up Questions	- Why is low atomic mobility benefical to the strength of a polymer? - What sort of additives can improve the dispersion of MMT? - How is the organic additive positioned relative to the particles in reality?

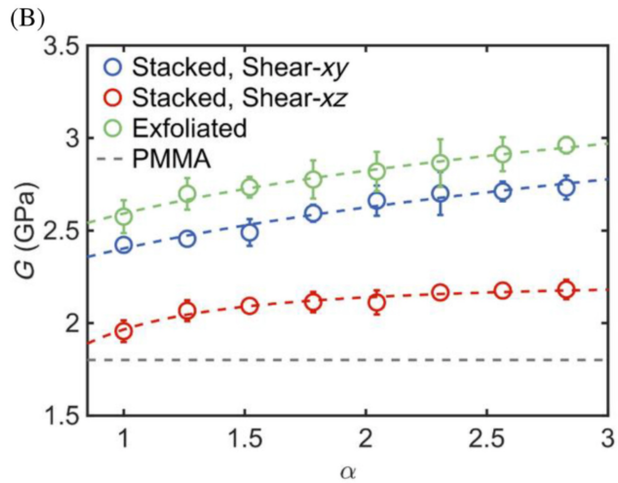
Article #20 Notes: 12/19/24 – Understanding the influence of configurations and intermolecular interaction on thermomechanical and dynamic properties of polymer–clay nanocomposites via molecular dynamics simulations.

Article notes should be on separate sheets

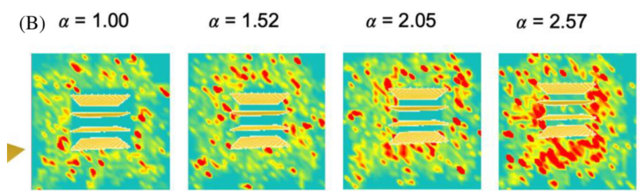
Source Title	Understanding the influence of configurations and intermolecular interaction on thermomechanical and dynamics properties of polymer–clay nanocomposites via molecular dynamics simulations
Source citation (APA Format)	Nie, W., Zhang, B., & Xie, D. (2024). Understanding the influence of configurations and intermolecular interaction on thermomechanical and dynamic properties of polymer–clay nanocomposites via molecular dynamics simulations. *Polymer Composites, 1*(15). https://doi.org/10.1002/pc.29303
Original URL	https://doi.org/10.1002/pc.29303
	Journal Article
Keywords	Polymer nanocomposites, Molecular dynamics, Mechanical properties.
#Tags	#composite, #nanoparticles, #MD
Summary of key points + notes (include methodology)	**Summary/Why It's important** - Polymer-clay nanocomposites are lightweight with exceptional thermomechanical properties, achieved by integrating clay nanofillers - PMMA is a popular polymer matrix - Exfoliated nanoclay structures are superior to stacked configurations - Nanoclay slows PMMA's global dynamics, with less influence farther from the clay layers - Nanoclay configuration affects PMMAs during deformation. **Notes** - Montmorillonite's high aspect ratio allows it to improve properties

	- Improvement of properties is limited by poor dispersion - Previous studies used stacked nanoclay layers –but those do not represent irregular exfoliated pattern in the real world - Coarse-grained (CG) modeling in this study allows exploration beyond experimental limitations. - Nanoclays affected stiffness of the polymer - **Methods/Results** - Coarse-grained models were 2-3x faster than alternatives while preserving molecular properties - Lennard-Jones potential was used for the simulation. - System is created with 665 PMMA chains and 10% nanoclay - energy minimization, annealing, and equilibration performed with MD simulations - Shear deformation analysis matched values from other experiments. - Exfoliated configurations have the highest shear modulus due to stronger polymer and nanoclay interaction - Shear modulus increases with interaction strength and temperature - Higher tensile modulus as well - As the interaction between nanoclay and polymer strengthens, interfacial stiffness increases, making the material more heterogeneous. - The study allows fine tuning and greater understanding of polymer nanocomposite materials.
Research Question/Problem/ Need	How does montmorillonite affect the properties of PMMA and other polymers, and how can this be modeled using MD simulations?
Important Figures	





Exfoliated structures have higher shear modulus and tensile modulus, even as a parameter alpha, representing intermolecular interactions, changes.

	 Red is more stiff and green is less. Local stiffness is higher around the clay layers.
VOCAB: (w/definition)	PMMA – popular polymer due to high impact resistance and mechanical properties used in various fields Coarse-grained modeling – simulation technique by grouping molecules into larger units called "beads"
Cited references to follow up on	- Zare et al., 2015, for general information on clay - Zhang et al., 2021, with a similar type of simulation
Follow up Questions	- How does the exfoliation of nanoclay affect thermal properties? - What role does the interaction strength between nanoclay and polymer have, and how can this be measured? - How do the simulation results for polymer clay nanocomposites compare to experimental data on similar materials?