

BACKGROUND

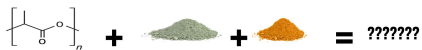
Plastic packaging made of traditional plastics pollutes the environment (Rosenboom et al., 2022).

PLA (polylactic acid) is a leading biodegradable alternative – but its mechanical/thermal properties are lacking (Gbadayan et al., 2024).



Clay nanoparticles increase strength of plastics (Uddin et al., 2024).

INNOVATION



- **Molecular dynamics** simulations accurately predict properties of polymers (Nikzad et al., 2024).
- **Can they save time/resources?**

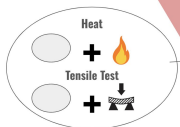
METHODS

5 types of nanoparticles
x 4 other types

Molecular dynamics (MD) simulations

Best composites

Real-world experimentation
1 bioplastic



Novel PLA Nanocomposite Bioplastic For Use In Packaging

Purpose

How do different forms of clay nanoparticles work together to affect the thermal and mechanical properties of polylactic acid?

Hypothesis

Different types of clay nanoparticles will increase mechanical strength and stiffness, as well as thermal resilience of PLA – beyond that of composites with each individual type and of pure PLA.

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Figure 1: Effect of volume fraction

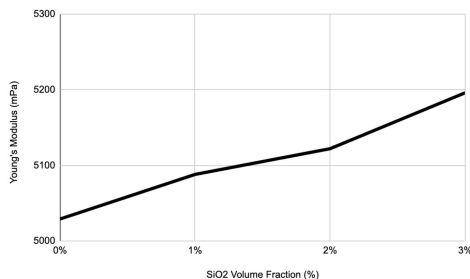


Figure 2: Simulation Equilibrium

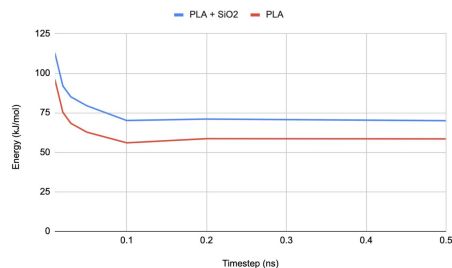


Table 1: Young's Modulus of PLA

| Young's Modulus (mPa) | |
|-------------------------------------|-------------|
| Experimental (Petsiuk et al., 2022) | Simulated |
| 1550 | 1491 |

ANALYSIS

Simulation reached equilibrium in terms of energy.

Young's Modulus of PLA matched values from previous experiments.

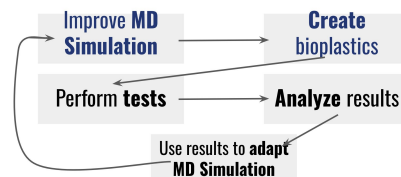
Young's Modulus vs. volume fraction of SiO2 forms a positive trend.

CONCLUSIONS

If the simulation is accurate, silicate nanoparticles may improve Young's Modulus of PLA.

Simulation is **grounded** in reality.

FUTURE STEPS



IMPORTANT REFERENCES

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