Analysis of Advanced Polymer Semiconductor Packaging Materials by Atomic Scale Simulation

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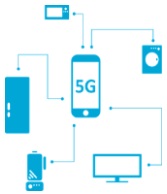
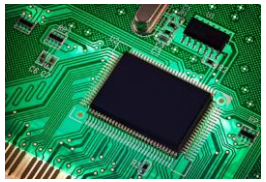
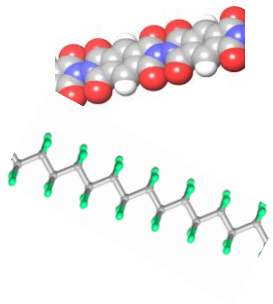
New Electronics Applications Require Advanced Packaging

Advancing Applications → **Demand** → **Next-Generation Chips** → **Require** → **Advanced Packaging Materials**



Next-generation wireless





Drive for improvements in electronic packaging require improved use of existing polymers and development of new polymers

Atomistic Modeling Provides a Toolset to Screen and Provide Insight in Polymer Design, Manufacturing, and Use

Use Case Example: Thermal Properties of Polymer Packaging

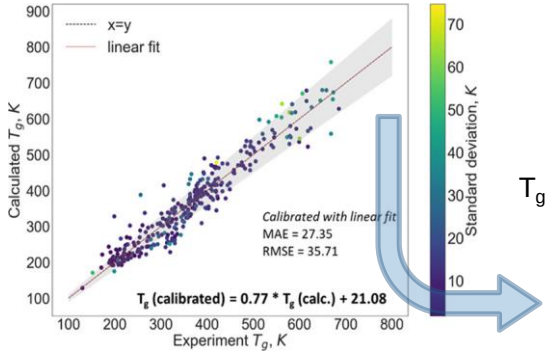
Devices performance is impacted by the behavior of packaging polymers at different temperatures. Critical packaging properties of glass transition and thermal stability can be evaluated using validated atomistic simulation techniques.

Device Changes with Temperature

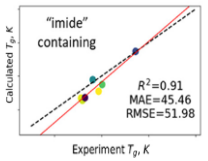
Glass Transition Temperature (Tg), Coefficient of Thermal Expansion

Molecular Dynamics simulation of dense polymer

Glass Transition Temperature (T_g)
for 300+ Polymers[1]
Predicted by MD Simulation[2]



T_g Prediction for imide-type polymers



GPU speed enabled high throughput simulation of > 3000 independent polymer cooling simulations

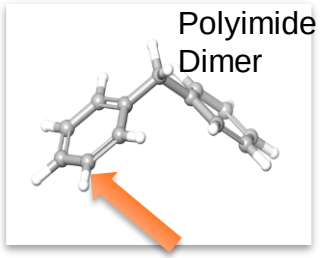
1 Experimental data taken from Bicerano, J., Prediction of Polymer Properties. Marcel Dekker Inc.: New York, 1996
2 Afzal, M. A. et al, ACS Appl. Polym. Mater., in press: https://doi.org/10.1021/acsapm.0c00524

Device Changes with Temperature

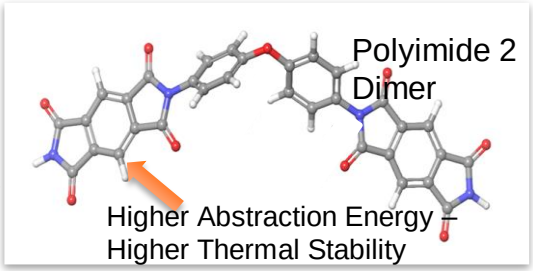
Thermal Stability

Quantum Mechanical simulation of hydrogen abstraction

Bond Dissociation Energy (BDE) provides insight into degradation mechanism packaging polymers.



Lower Abstraction Energy –
Lower Thermal Stability



Higher Abstraction Energy –
Higher Thermal Stability

Structure	BDE /(kcal/mol)	Full Degradation Modeling ΔG_{eff} (1) /(kcal/mol)
Polyimide 1	85.8	54.5
Polyimide 2	121.2	81.3

Increase Energy –
Increase Thermal Stability

Fast BDE Calculations provided same insight in thermal stability as full Quantum Mechanism mapping

1. Kunnikuruvan, S., et al *Macromol Theor Simul.* **24**,4, 2014, 344-351

Use Case Example: Mechanical and Chemical Properties of Polymer Packaging

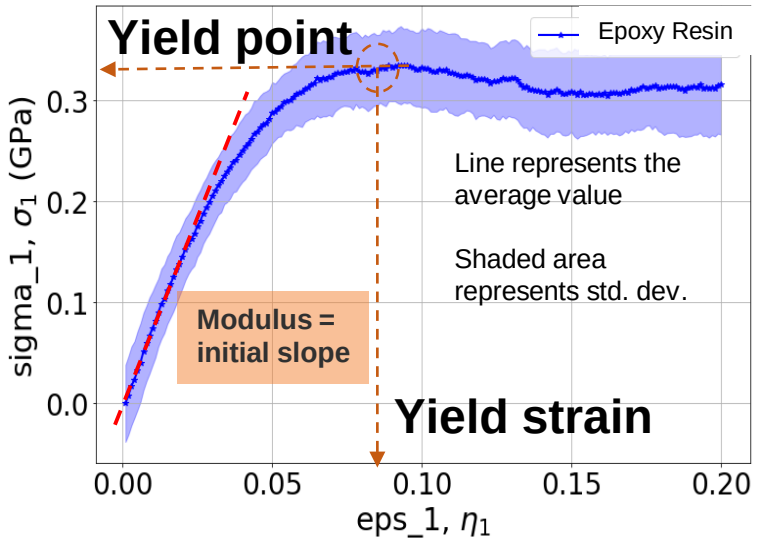
Devices performance is impacted by the mechanical properties and the chemical performance of packaging polymers. Atomistic simulation can provide these properties as well as a connection to specific molecular group behavior for improved polymer design.

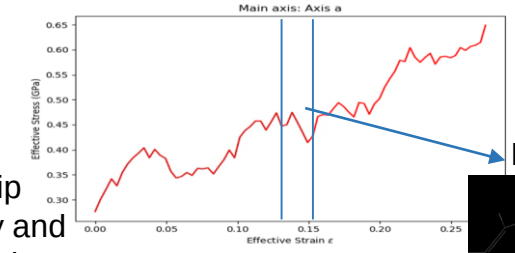
Device Defection and Strength

Modulus, Tensile Yield

Molecular Dynamics simulation of dense polymer

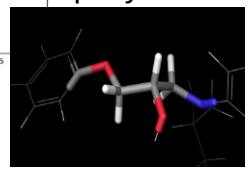
Explore Overall Property through Aggregate Curve





Explore Relationship Between Chemistry and Property by Detailed Analysis of Simulations

Epoxy Resin



molecule flip corresponds to stress drop

Device Lifetime

Water Absorption, Chemical Resistance

Molecular Dynamics simulation of water loading and solvent ingress

Equilibrium Water Uptake in Epoxy Resin Formulations

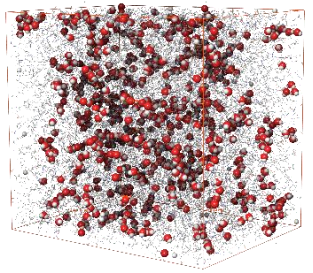
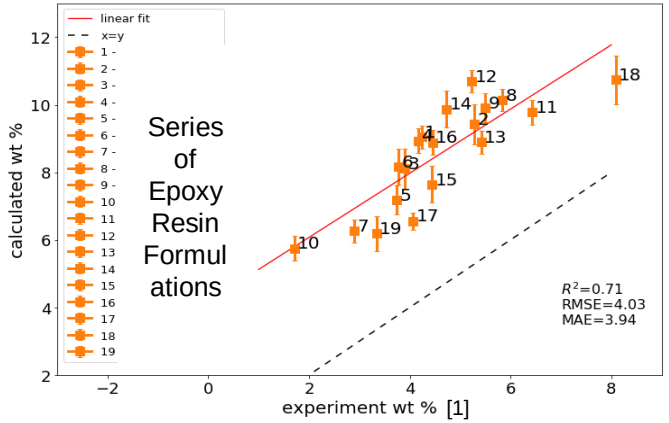


Image of fully water loaded epoxy resin
Epoxy resin – gray dots
Water – red/white sphere



1. Frank, Katherine Lea. "Relationships between cure kinetics, network architecture, and fluid sensitivity in glassy epoxies.“, Thesis University of Southern Mississippi. 2013.

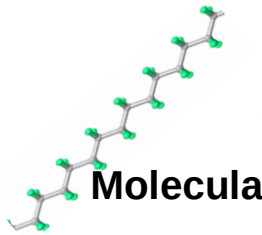
Use Case Example: Electrical and Optical Properties of Polymer Packaging

Packaging polymers must meet electrical properties of dielectric constant and loss requirements to be useful in devices. Atomistic simulation can provide these properties via combination of simulation techniques.

Device Loss and Dissipation

Dielectric Loss

Molecular Dynamics simulation of polymer oligomers



Molecular Quantum mechanics

Molecular structure

Polarizability

Automated dipole sampling and frequency analysis

OUT

Refractive index

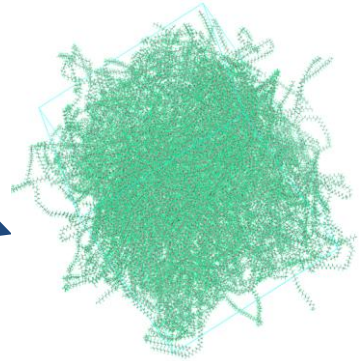
Dielectric constant (ε)

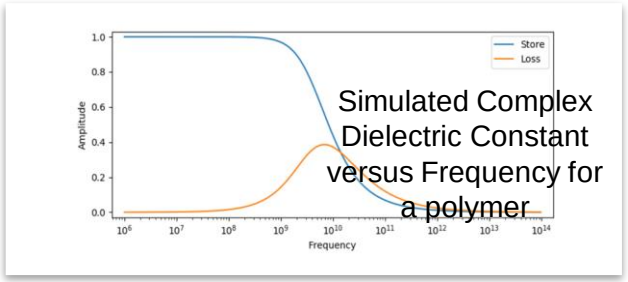
Dielectric loss (ω)

OUT

Bulk Density

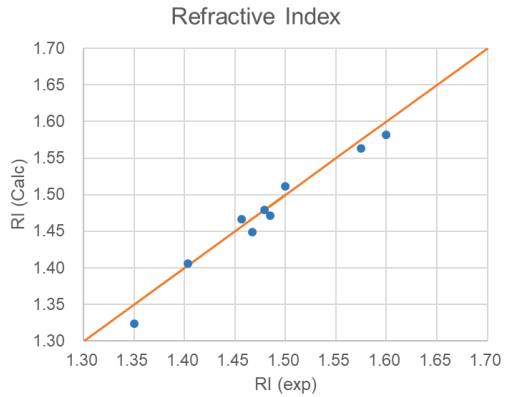
Automated model building & Molecular Dynamics equilibration

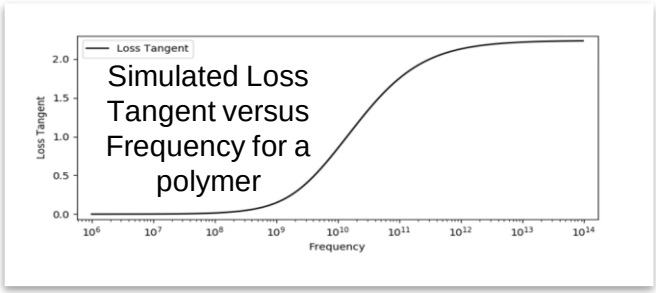




Simulated Complex Dielectric Constant versus Frequency for a polymer

Predicted Refractive Index versus Experiment for Series of Homopolymers

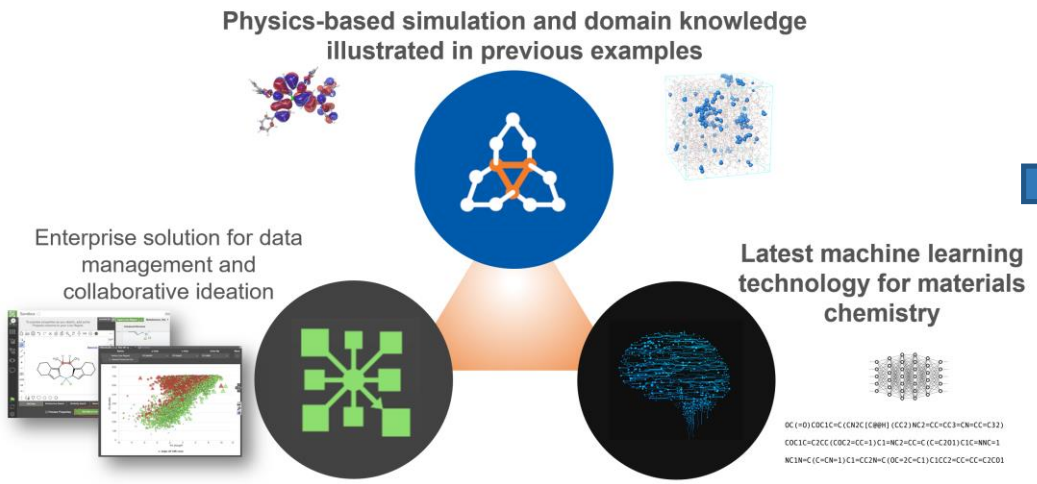




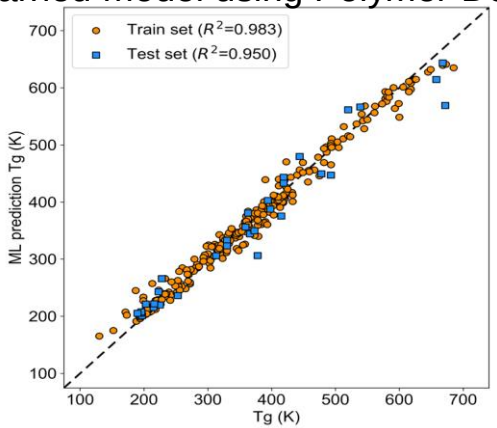
Simulated Loss Tangent versus Frequency for a polymer

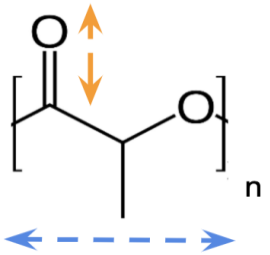
Machine Learning Leverages Data for Prediction Across Polymer Packaging Requirements

Machine learning techniques can be applied in combination with physics based simulation or experimental datasets to provide fast evaluation of properties for materials design applications.



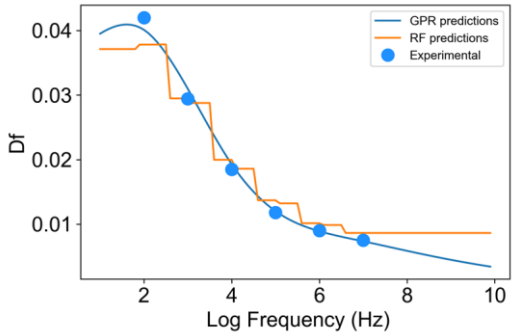
Example: Glass Transition Temperature Machine Learned model using Polymer Descriptors





Polymer descriptors capture features of polymers better than molecular based descriptors.

Example: Frequency dependent prediction of tan delta (Df) using ML models



Machine Learning predictions (two approaches)