Material Property Simulation for Advanced Packaging

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21ST INTERNATIONAL CONFERENCE & EXHIBITION ON DEVICE PACKAGING
SHERATON GRAND AT WILD HORSE PASS PHOENIX, AZ
MARCH 3-6, 2025 • WWW.DEVICEPACKAGING.ORG

Outline

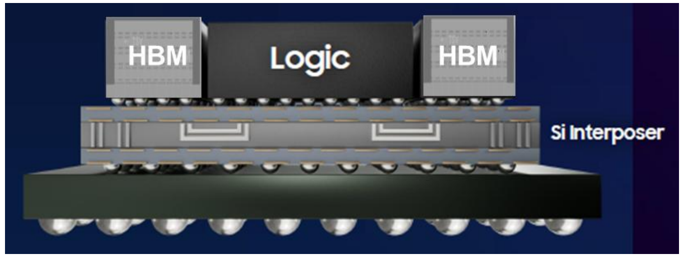
- Introduction
- Molecular Simulation (based on quantum mechanics, molecular dynamics and machine learning)
- Example of Calculation
- PID Material Property Calculation
- Challenges
- Conclusion and Next Plan

Introduction

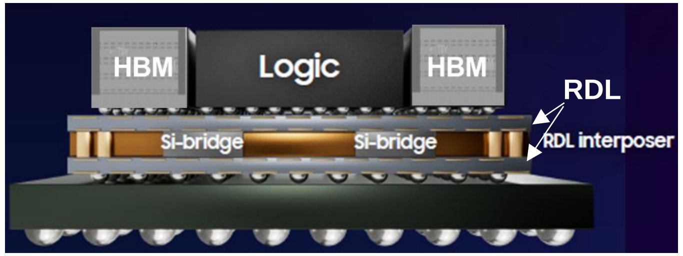
https://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=10195617

Advanced packages on market

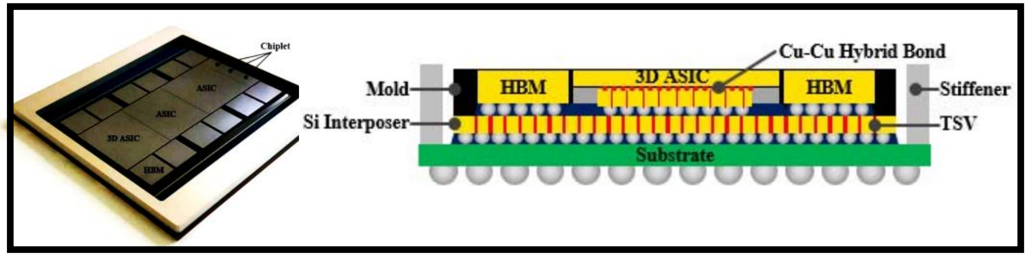
Smaller interconnects; Higher performance; Lower power consumption



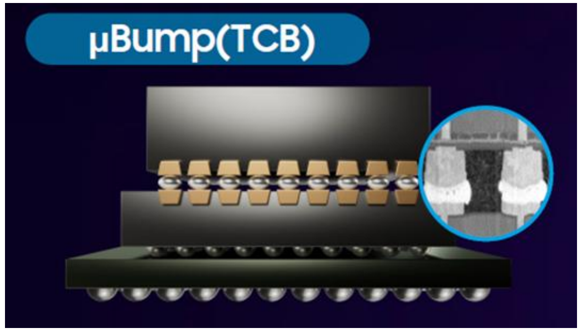
I-Cube S: Si interposer from Samsung



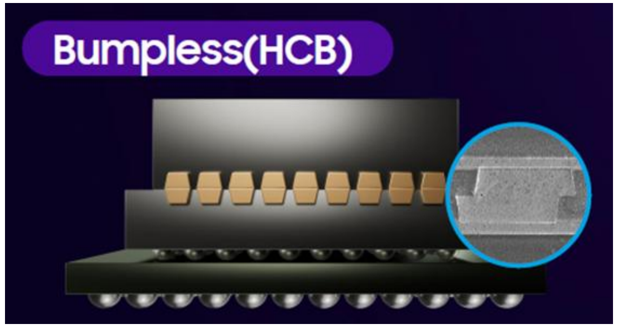
I-Cube R/E: Redistribution Layer (RDL) interposer (I-cube R) with the option of Embedded Si bridge (I-cube E) from Samsung



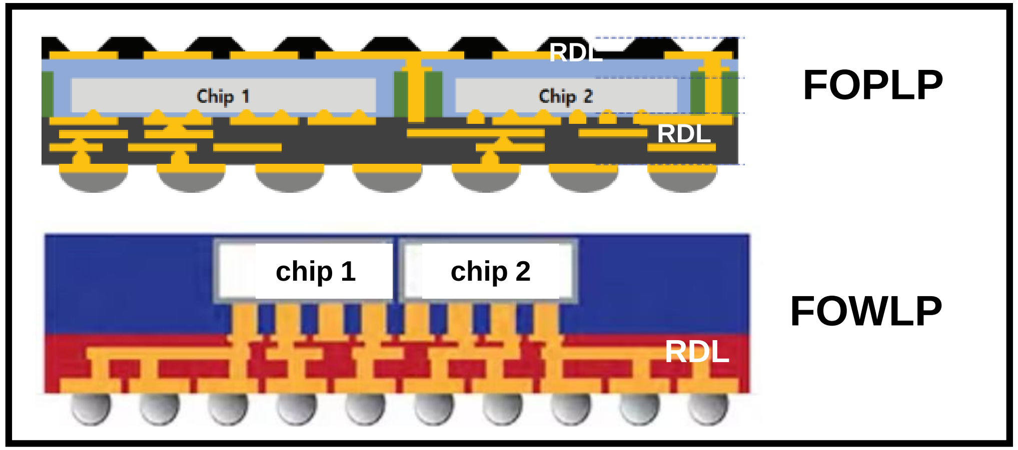
3.5D packaging: hybrid bonding 3D chips on Si interposer from Samsung



X-Cube: logic to logic die stacking- µBump from Samsung



X-Cube: logic to logic die stacking- Hybrid Cupper Bonding Samsung



https://ieeetv.ieee.org/video/heterogeneous-integration-platform-for-next-generation-computing-beyond-moore

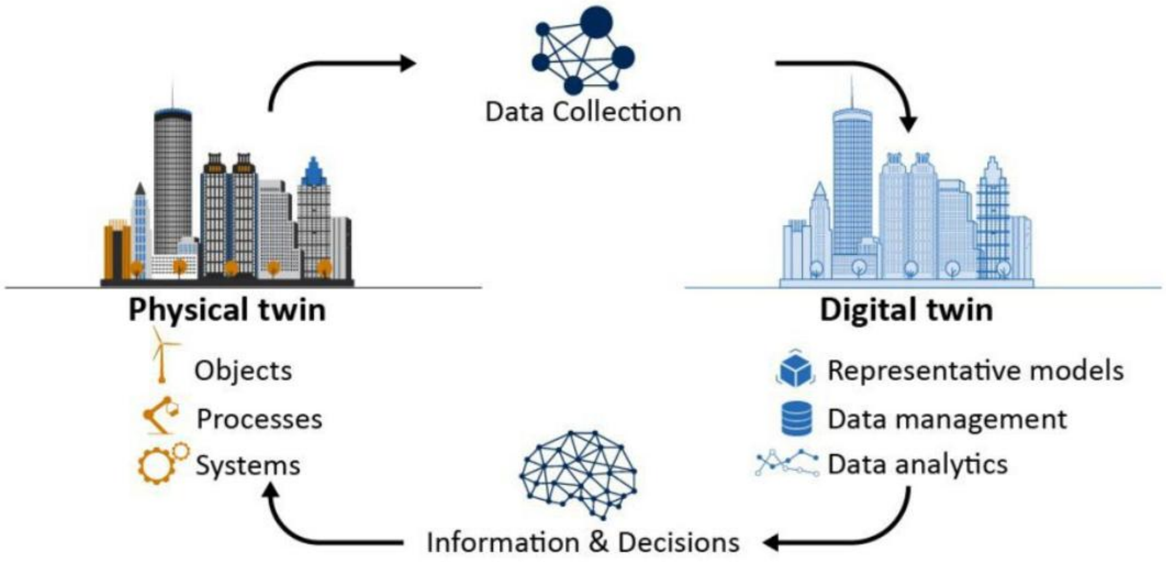
W. Kim, “Advanced Packaging in the Era of HPC and AI” Seventh Annual Symposium on Heterogeneous Integration, February, 2024.

Introduction

- Adopting AI based methodologies to advanced packaging

- The key for an accurate simulation model is to input precise material properties

- Material property simulation of organic packaging materials



Sources: GAO; ladoga/stock.adobe.com. | GAO-23-106453

Introduction

Material property simulation of PID

Undulation or non-planarity during Multilayer Patterning

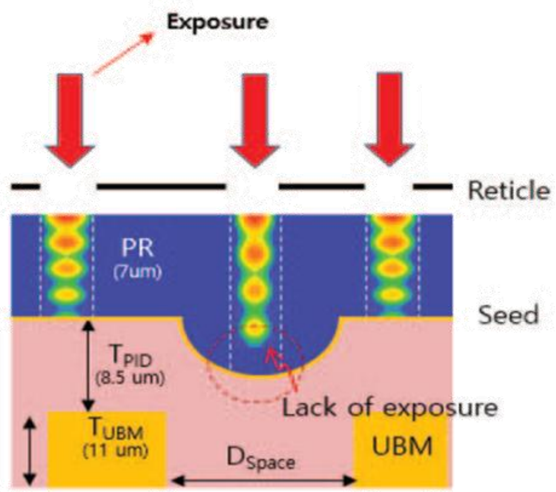


Figure 5. Assumed mechanism of open failure by the undulation of dielectric

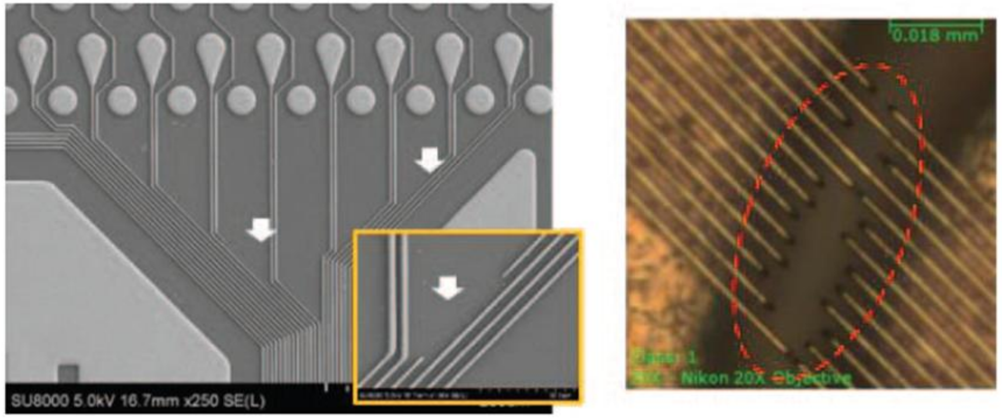


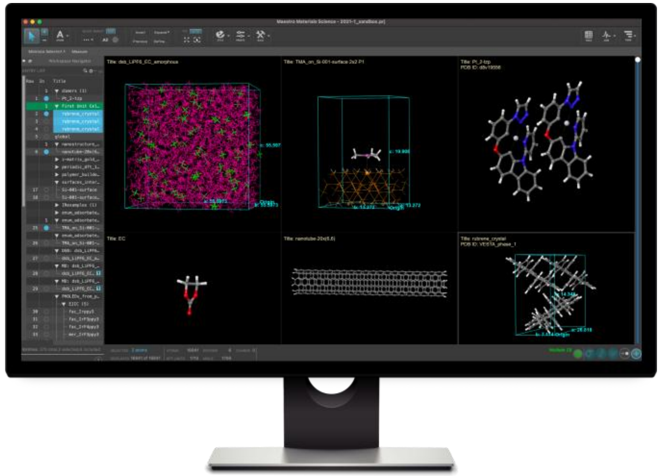
Figure 4. Top view SEM and OM images of open failure after seed etch

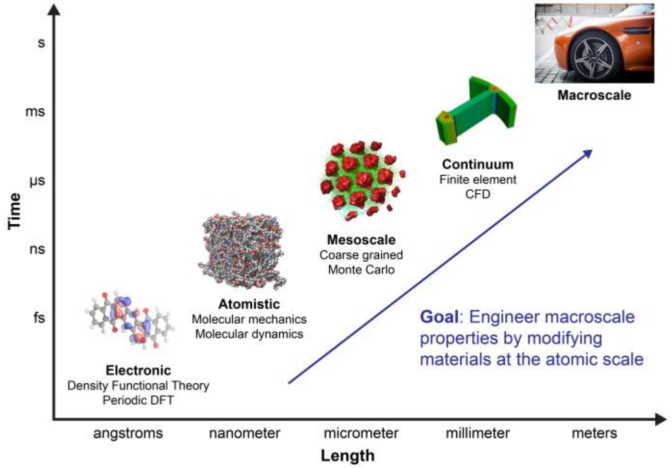
Open failures due to undulation in the Photo Imageable Dielectric layer (PID), which is caused by PID shrinkage during curing

Y. Kim et. al. 2021 IEEE 71st Electronic Components and Technology Conference (ECTC)

Molecular Simulation

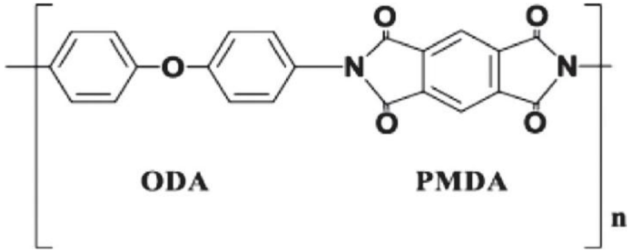
Schrödinger platform



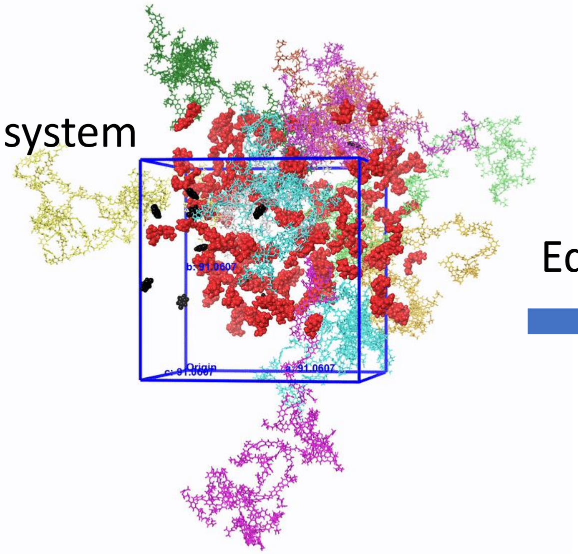


Goal: Engineer macroscale properties by modifying materials at the atomic scale

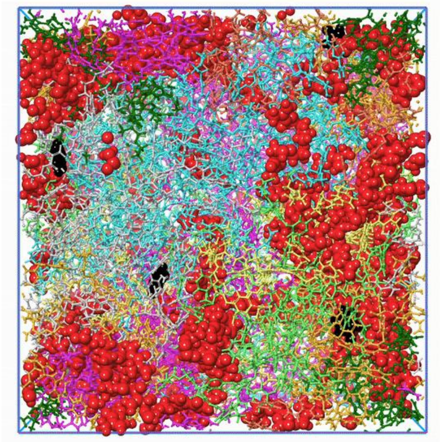
Example system of interest



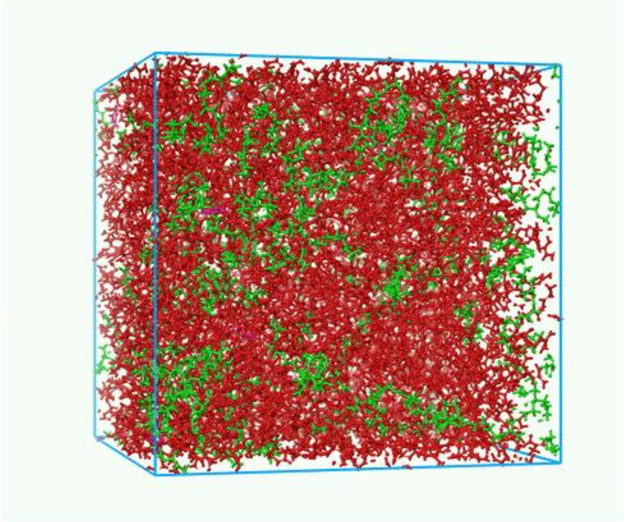
Initial system



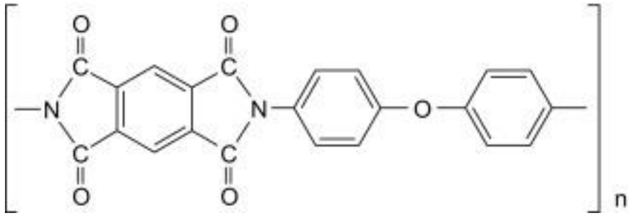
Equilibration



Crosslinking



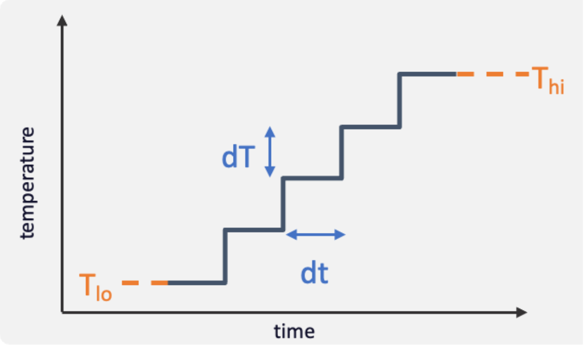
Example of Calculation (T_g using MD)



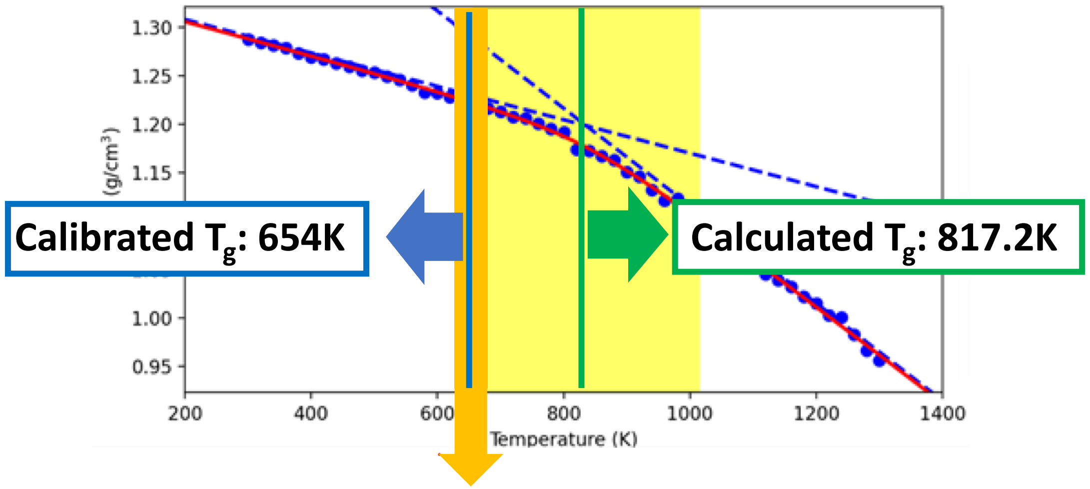
Kapton®

Simulation settings:

- dT → 10 K
- dt → 5 ns
- (T_{hi}, T_{lo}) → (1300 K, 300 K)



Calculated T_g results

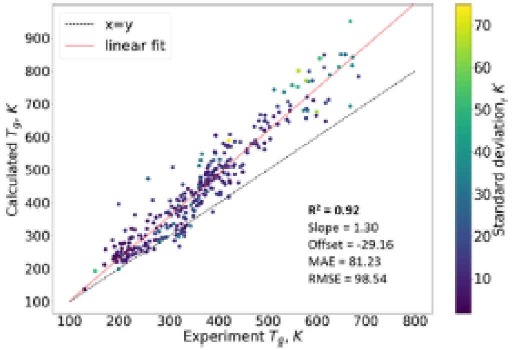


Calibrated T_g: 654K

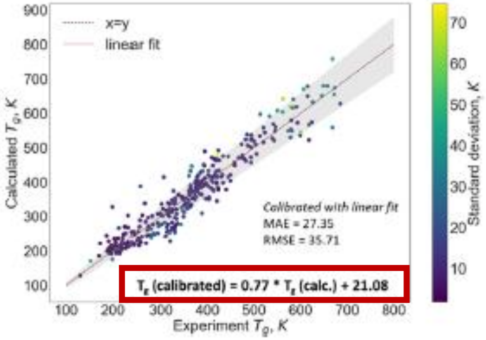
Calculated T_g: 817.2K

Experimental T_g: 633K – 683K *

Validation of the Schrödinger T_g protocol



Predicted T_g values against experimental ones reported in Bicerano, Table 6.2.



Calibrated T_g values against experimental ones reported in Bicerano, Table 6.2.

Mohammad Atif Faiz Afzal *et al.* ACS *Appl. Polym. Mater.* 2021, 3, 620-630

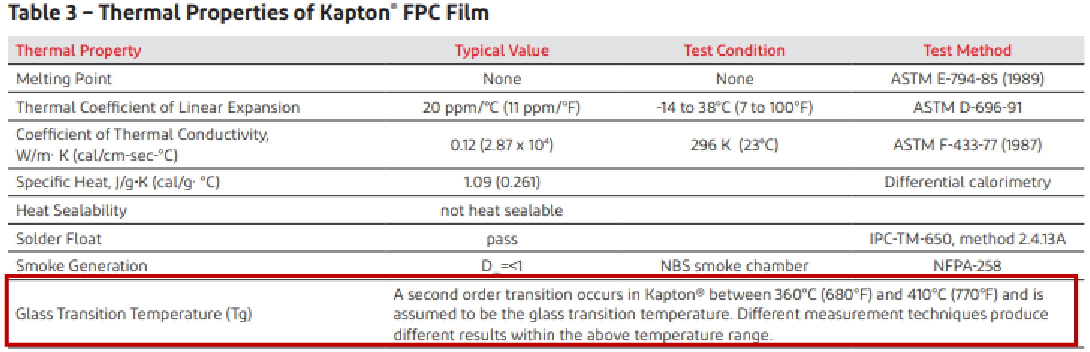


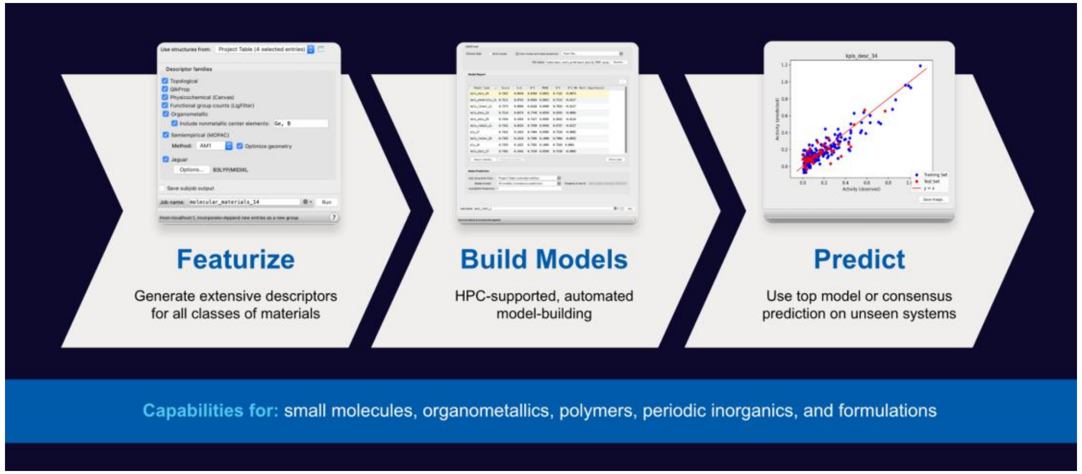
Table 3 – Thermal Properties of Kapton® FPC Film

Thermal Property	Typical Value	Test Condition	Test Method
Melting Point	None	None	ASTM E-794-85 (1989)
Thermal Coefficient of Linear Expansion	20 ppm/°C (11 ppm/°F)	-14 to 38°C (7 to 100°F)	ASTM D-696-91
Coefficient of Thermal Conductivity, W/m· K (cal/cm-sec-°C)	0.12 (2.87 x 10^4)	296 K (23°C)	ASTM F-433-77 (1987)
Specific Heat, J/g·K (cal/g· °C)	1.09 (0.261)		Differential calorimetry
Heat Sealability	not heat sealable		
Solder Float	pass		IPC-TM-650, method 2.4.13A
Smoke Generation	D_m =<1	NBS smoke chamber	NFPA-258
Glass Transition Temperature (Tg)	A second order transition occurs in Kapton® between 360°C (680°F) and 410°C (770°F) and is assumed to be the glass transition temperature. Different measurement techniques produce different results within the above temperature range.		

* Dupont Kapton Summary of Properties
https://www.dupont.com/content/dam/electronics/amer/us/en/electronics/public/documents/en/EI-10142_Kapton-Summary-of-Properties.pdf

Example of Calculation (T_g using ML)

Schrödinger machine learning workflow for materials



Featurize

Generate extensive descriptors for all classes of materials

Build Models

HPC-supported, automated model-building

Predict

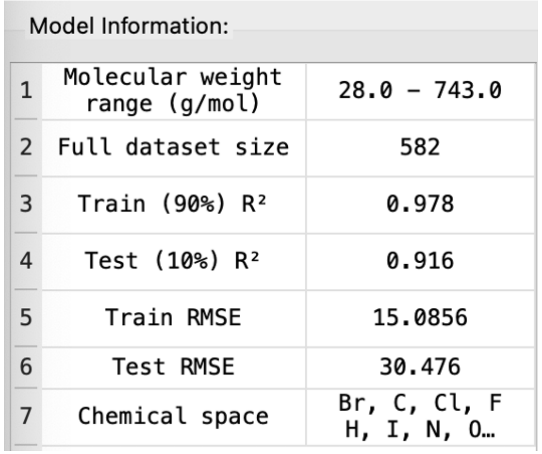
Use top model or consensus prediction on unseen systems

Capabilities for: small molecules, organometallics, polymers, periodic inorganics, and formulations

Property prediction using Schrödinger pre-built ML models trained using experimental data.

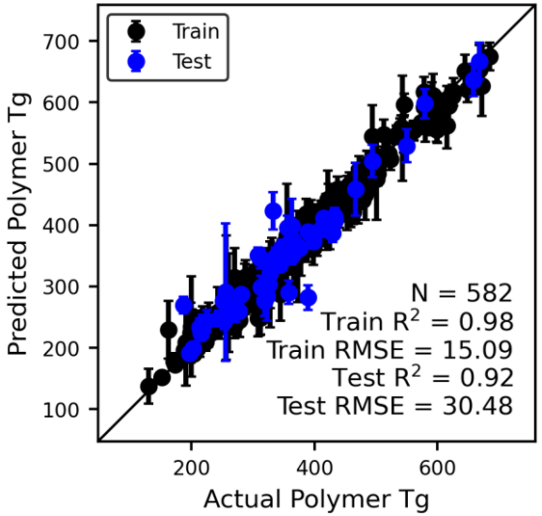
Property prediction in a fraction of section!

Tg machine learning model

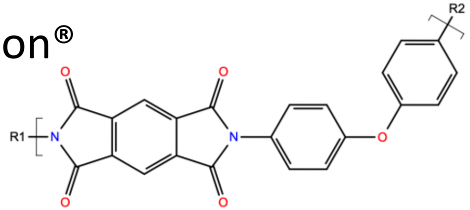


Model Information:

1	Molecular weight range (g/mol)	28.0 – 743.0
2	Full dataset size	582
3	Train (90%) R²	0.978
4	Test (10%) R²	0.916
5	Train RMSE	15.0856
6	Test RMSE	30.476
7	Chemical space	Br, C, Cl, F H, I, N, O…



Kapton®



Predicted Tg → 633.1 K

Kapton®: Experiment Tg is 672K from Bicerano*

*Bicerano, Jozef. *Prediction of polymer properties*. cRc Press, 2002.

Molecular Simulation: Mechanical Properties

Simulation settings:

- Stress based calculation
- Uniaxial and biaxial tension
- Temperature → 330 K
- Simulation time → 100 ns
- Strain of 0.2% for 8 steps in a, b, c directions

$$\boldsymbol{\sigma} = \boldsymbol{C\epsilon}$$

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ 2\epsilon_5 \\ 2\epsilon_5 \\ 2\epsilon_6 \end{bmatrix}$$

- Properties from the workflow
  - Universal Anisotropy, Shear Anisotropy, Lamé Lambda, Lamé Mu, Young's Modulus, Shear Modulus, Lamé Bulk Modulus, Poisson Ratio

Calculated properties

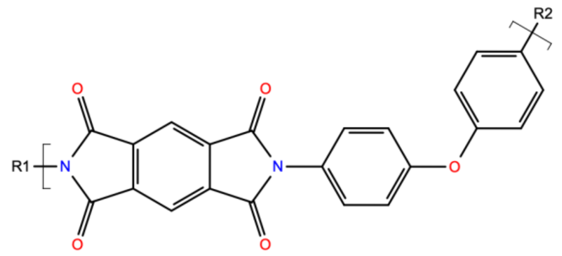
Young's modulus (MPa): 2423

Bulk modulus (MPa): 4497

Shear modulus (MPa): 859

Universal elastic anisotropy: 0.497

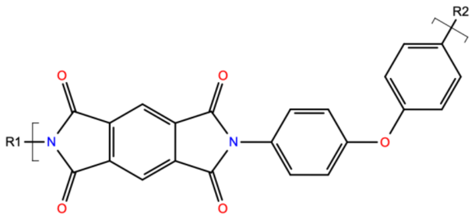
Isotropic Poisson ratio: 0.410



Exp. Young's Modulus → 2760 MPa

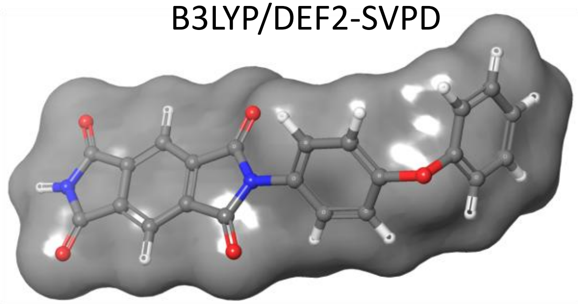
Molecular Simulation: Dielectric Properties

Example polymer structure



Quantum mechanics (Density functional theory)

B3LYP/DEF2-SVPD



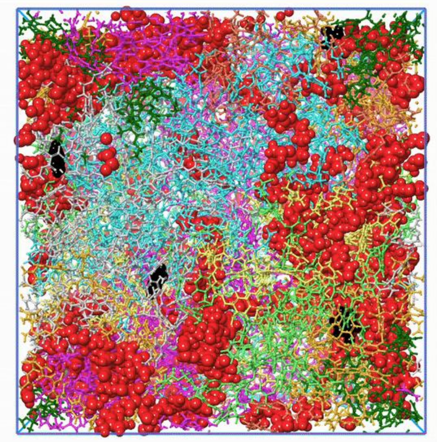
Polarizability

Physics-based Dk, Df, and RI

Density + Dipole moment

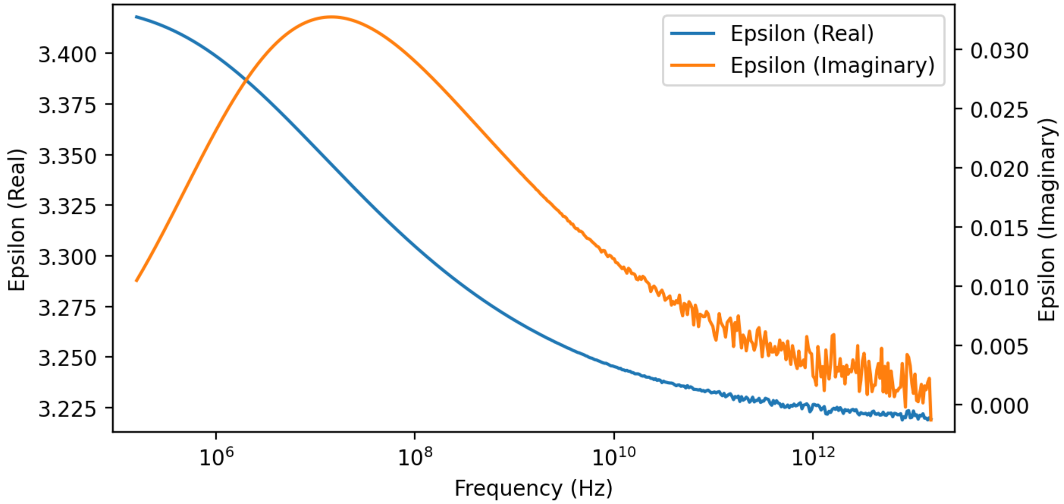
Molecular dynamics simulations

Time: 50 ns
Ensemble: NVE
T: 300 K
Chain length:
27 monomer



Calculated properties

RI → 1.79
Dk (at 10^{10} Hz) → 3.25
Df (at 10^{10} Hz) → 0.012



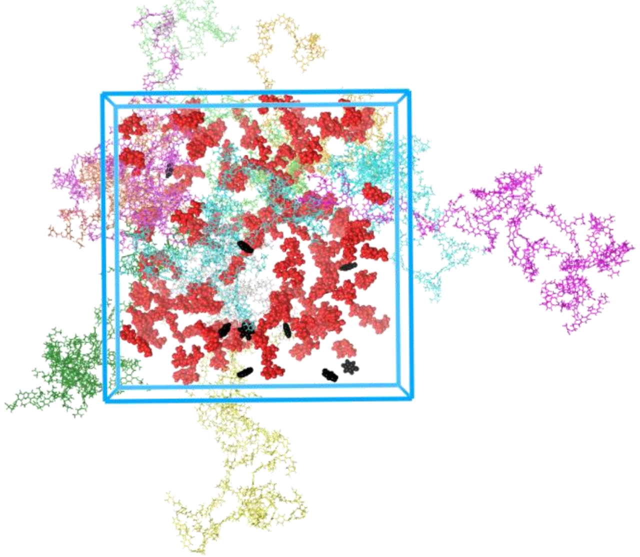
Molecular Simulation: Volume Shrinkage

Simulation settings:

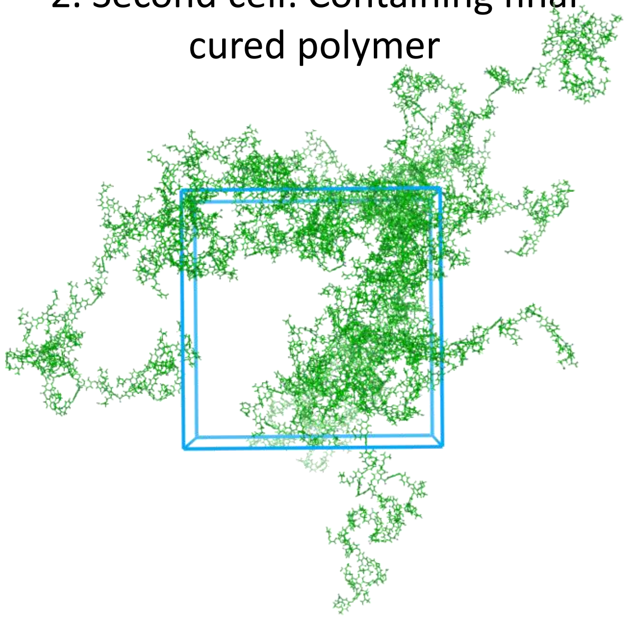
- Simulate two systems
  - First simulation cell: precursor + photo initiator + crosslinker
  - Second simulation cell: pure PI system after curing
- Keep polymer stoichiometry same in both system

- Perform multi-stage simulation at 300K and obtain equilibrated structure
- Take volume % change between 1 and 2

1. First cell: Containing precursor, crosslinker and photo initiator



2. Second cell: Containing final cured polymer



PID Material Property Calculations

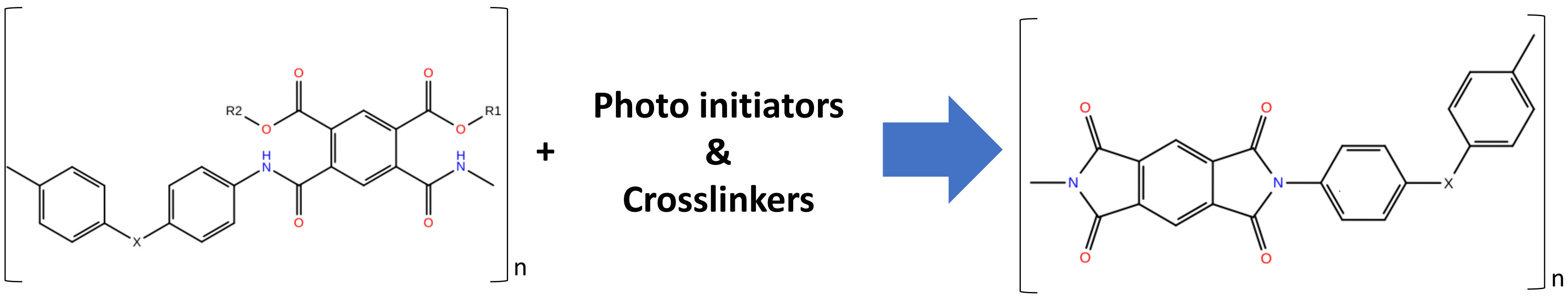
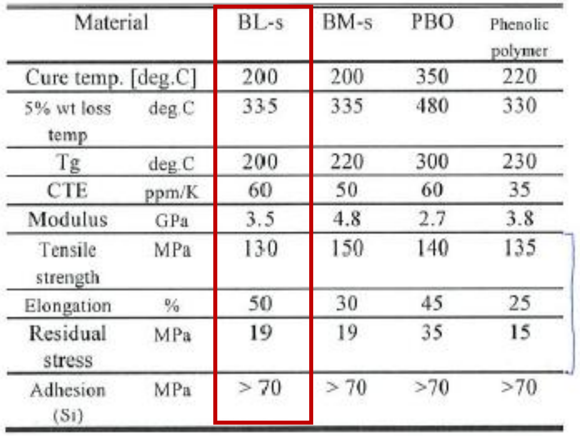


Photo initiators
&
Crosslinkers

PI precursor structure before curing

PI structure before curing

- Kept polymer stoichiometry same in both systems.
- Equilibrium at room temperature.
- Volume change of 37% vs. 30% of experimental value



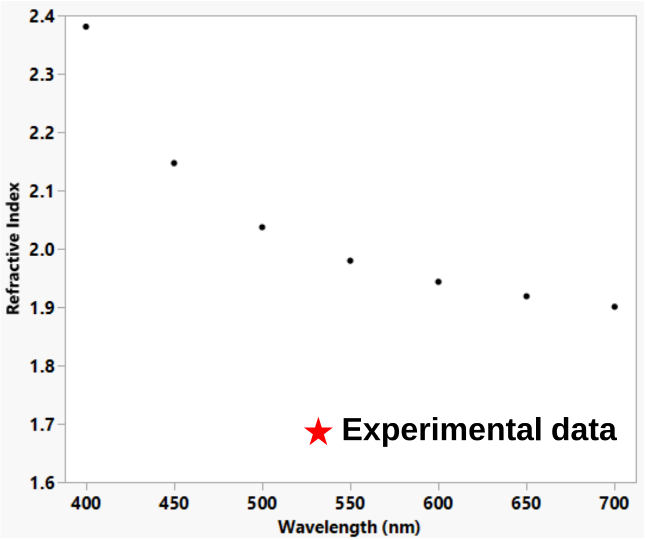
Material		BL-s	BM-s	PBO	Phenolic polymer
Cure temp. [deg.C]		200	200	350	220
5% wt loss temp	deg.C	335	335	480	330
Tg	deg.C	200	220	300	230
CTE	ppm/K	60	50	60	35
Modulus	GPa	3.5	4.8	2.7	3.8
Tensile strength	MPa	130	150	140	135
Elongation	%	50	30	45	25
Residual stress	MPa	19	19	35	15
Adhesion (Si)	MPa	> 70	> 70	>70	>70

Table 1. Typical properties of dielectric material

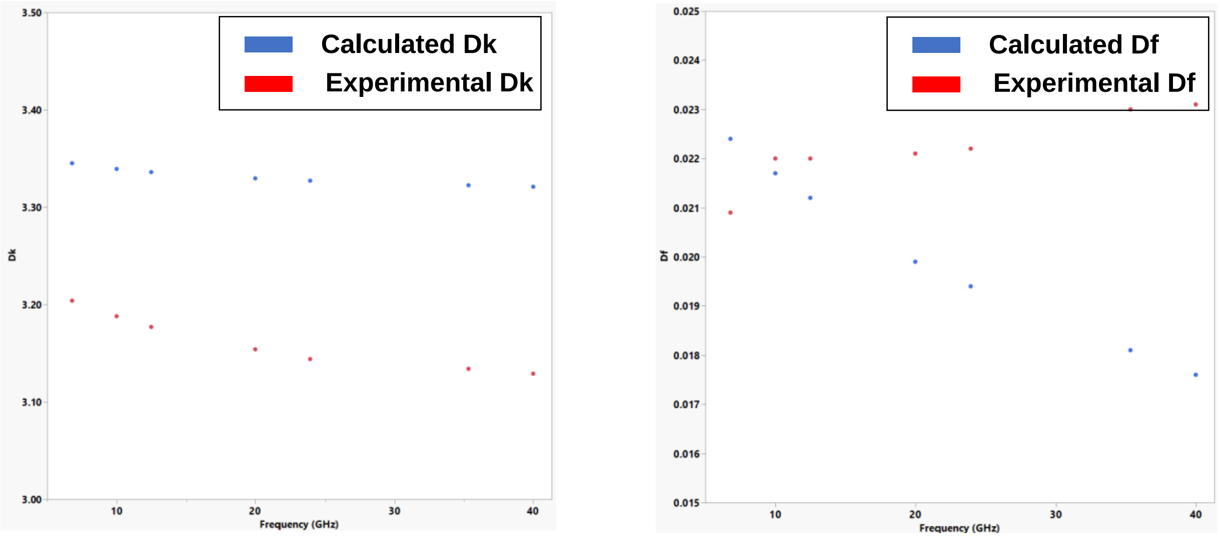
Nobuhiro Anzai *et, Proc. IEEE Electronic Components & Technology Conference*, 2014, 829-835

PID Material Property Calculations

Refractive Index

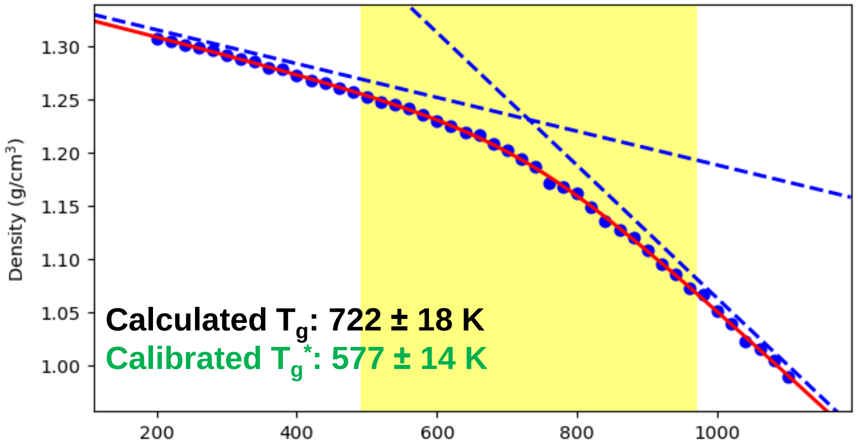


Dielectric constants



Properties	Discrepancy to the experimental values
T_g	Up to 18%
D_f	Up to 6%
D_k	Up to 23%
Young’s modulus	~15%
Refractive Index	16% at 530nm wavelength
Volume shrinkage	~18%

Glass Transition Temperature



Calculated T_g: 722 ± 18 K

Calibrated T_g^*: 577 ± 14 K

Challenges

- **Bridging the gap between simulation data and experiment data**
  - Narrowing the 6%-23% difference between simulation and experiment.
  - Accounting for density and functional groups.
  - Integrating formulated materials into models could give better experimental alignment.

Next Step: Include the impact of additional ingredients or impurities in simulation

Conclusion and Next Plan

- Simulation and AI assisted process optimization, yield and reliability prediction to shorten product development cycle time.
- Accurate material properties under test conditions are crucial.
- Need to establish reliable material simulation methodology.