

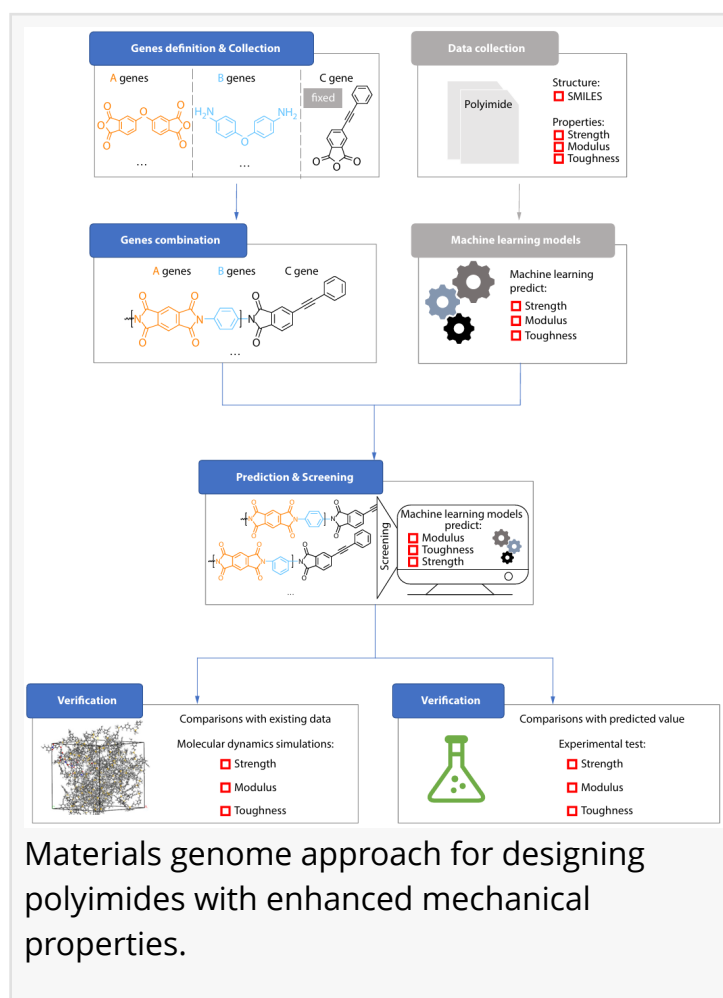
AI-driven genome strategy accelerates design of ultra-tough polyimide films

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/EINPresswire.com/ -- Balancing stiffness, strength, and toughness in thermosetting polyimide films has long challenged materials scientists. In this study, researchers combined machine learning with a materials-genome framework to rapidly predict and optimize these competing properties. By defining polymer substructures as molecular "genes," they screened more than 1,700 phenylethynyl-terminated polyimide candidates and identified one formulation, PPI-TB, with simultaneously high Young's modulus, tensile strength, and elongation at break. The model's predictions were confirmed by molecular dynamics simulations and laboratory testing. This integrated strategy drastically shortens development cycles and provides a cost-effective, data-driven pathway for designing high-performance polymer films.

Polyimide films are essential in aerospace, flexible electronics, and micro-display technologies for their thermal stability and insulation. However, mechanical optimization remains elusive: high modulus often reduces toughness, and improving one property tends to compromise another. Traditional trial-and-error synthesis is slow, costly, and limited in exploring complex molecular spaces. The rise of materials-genome approaches—integrating computation, experiment, and AI—offers a solution by learning structure–property relationships directly from data. Yet, most prior models addressed single properties or small datasets. Due to these challenges, a systematic, high-throughput strategy is urgently needed to design polyimides with superior, well-balanced mechanical performance.

A research team from the East China University of Science and Technology has developed an AI-assisted materials-genome approach (MGA) that enables the rapid design of high-performance



thermosetting polyimides. Their study, published online on September 2, 2025, in the Chinese Journal of Polymer Science, introduces a machine-learning model capable of predicting three key mechanical parameters—Young's modulus, tensile strength, and elongation at break—across thousands of candidate structures. The approach successfully identified a new formulation, PPI-TB, whose performance surpassed well-known benchmark polyimides.

The team constructed [Gaussian process regression](#) (GPR) models trained on over 120 experimental datasets of polyimide films. Each polymer's structural fragments—dianhydride, diamine, and end-capping units—were treated as "genes," defining a vast chemical space of 1,720 phenylethynyl-terminated polyimides (PPIs). The models achieved high predictive accuracy ($R^2 \approx 0.70$ – 0.74) for all three mechanical metrics and were used to score every candidate for comprehensive mechanical performance. Molecular dynamics simulations validated the screening, showing that PPI-TB (gene combination A□/B□□) exhibited superior modulus (3.48 GPa), toughness, and strength indicators compared with established systems PETI-1 and O-O-3. Subsequent experiments on representative PPIs confirmed the strong consistency between predicted and measured data.

Further "gene" and feature-importance analyses revealed key design principles: conjugated aromatic structures enhance stiffness, heteroatoms and heterocycles strengthen molecular interactions, and flexible Si- or S-containing units improve elongation. Together, these insights demonstrate how integrating AI predictions with molecular interpretation can uncover structure–property rules and accelerate polymer innovation.

"By translating polymer fragments into genetic-like descriptors, we can treat molecular design like decoding a genome," said Prof. Li-Quan Wang, one of the corresponding authors of the study. "Machine learning not only predicts performance but also reveals which chemical 'genes' are driving it. This synergy between data science and chemistry allows us to explore material possibilities that would take decades by conventional means. The success of PPI-TB exemplifies how AI can redefine the discovery process for next-generation high-temperature polymers."

The AI-driven materials-genome strategy provides a universal, scalable framework for designing polymers with targeted combinations of stiffness, strength, and flexibility—traits essential to microelectronics, aerospace composites, and flexible circuit substrates. By replacing years of experimental iteration with predictive modeling and virtual screening, this method drastically reduces cost and development time. Beyond polyimides, the workflow could be adapted for other high-performance polymer classes, guiding the creation of lightweight, durable, and thermally stable materials that power future electronic and aerospace technologies.

References

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