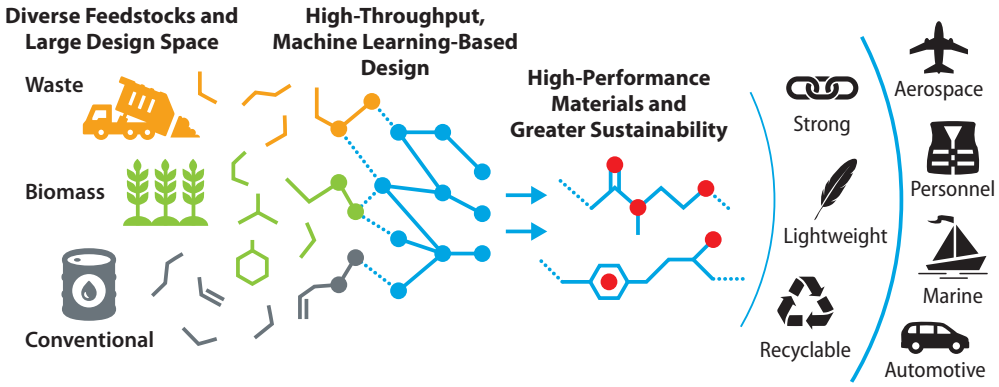
NREL Transforming ENERGY

U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY
BIOENERGY TECHNOLOGIES OFFICE

Accelerating Materials Discovery:
Artificial Intelligence for Sustainable, High-Performance Polymers

PolyID
Polymer Inverse Design

Heat-resistant vehicle parts; stronger and lighter personal protective equipment; recyclable and leak-proof food packaging—the quality and performance of today's commodities hinge on the basic materials from which they are made. Developed with support from the U.S. Department of Energy Bioenergy Technologies Office, **PolyID: Polymer Inverse Design™** revolutionizes materials discovery by making it faster and easier to find sustainable and high-performance polymers for a given application.

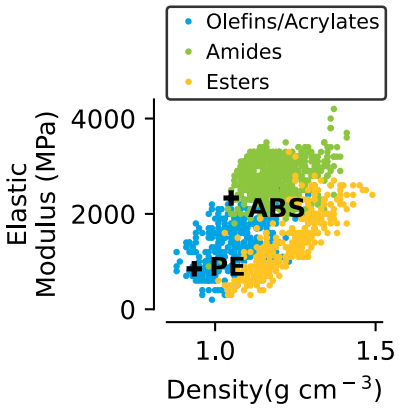


Beyond Trial and Error

It can be daunting to choose the correct polymer for high performance from among millions of unique materials that can be made from biomass, waste, and conventional feedstocks. PolyID™ uses graph neural networks to predict materials properties based on molecular structure. This offers distinct advantages to the materials discovery process:

1. Advanced Performance

PolyID predicts material properties from molecular structure so researchers can identify materials with the best performance. For example, the tool screened ≥22,000 polymers to pinpoint candidates that are lighter, stronger, stiffer, and less dense (see figure to the right).



2. Faster Development

As a high-throughput machine learning tool, PolyID can screen millions of possibilities into a short list of ideal candidates for a given application.

3. Improved Sustainability

PolyID centers a range of sustainability factors in the materials development process, such as:

- Greenhouse gas emissions
- Supply chain energy
- Water use
- Reuse of embedded energy and mass
- Biodegradability
- Recyclability

Contact Us

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