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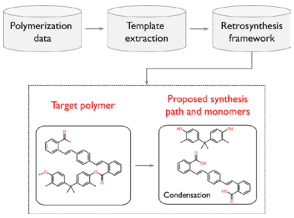
Using machine learning and data for over 11,000 polymers, researchers created a model to speed up the synthesis of new polymers.



Polymers have become a key class of materials in modern day life. From garbage bags to auto parts, polymers are designed for a wide range of uses.

But designing and synthesizing new polymers has historically required extensive knowledge, intuition, and time. An artificial intelligence algorithm, described in Chen et al., hopes to streamline that process.

The AI algorithm stems from previous polymer informatics work, which created the Polymer Genome, an online tool, where researchers can input a polymer and instantaneously predict dozens of its properties, paving the way for the intelligent design of polymers with desired characteristics. The authors detailed the next step in this process, which aims to help researchers figure out methods for making new polymers.

Using a data-driven approach, the authors collected synthesis information for over 11,000 existing polymers and analyzed the data with machine learning to create a model that provides synthesis recommendations for new polymers. For a given polymer, the model outputs the polymerization mechanism and the monomers required for synthesis.

In future iterations of the model, the authors hope to include other aspects of synthesis such as catalysts, initiators, temperature, and monomer concentration.

“This work is an important step for machine-assisted polymer synthesis,” said author Rampi Ramprasad. “But it’s still a first step, because there are so many more aspects of synthesis that need to be considered.”

The authors hope their model can someday be used in artificial intelligence-driven labs that can design, synthesize, and test polymers autonomously. In the meantime, they plan for the resource, which is now online at polymergenome.org, to be used as a digital assistant for synthetic chemists.

Source: “Data-assisted polymer retrosynthesis planning,” by Lihua Chen, Joseph Kern, Jordan P. Lightstone, and Rampi Ramprasad, *Applied Physics Reviews* (2021). The article can be accessed at https://doi.org/10.1063/5.0052962.

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