New automated platform accelerates discovery of high-performing polymer material blends

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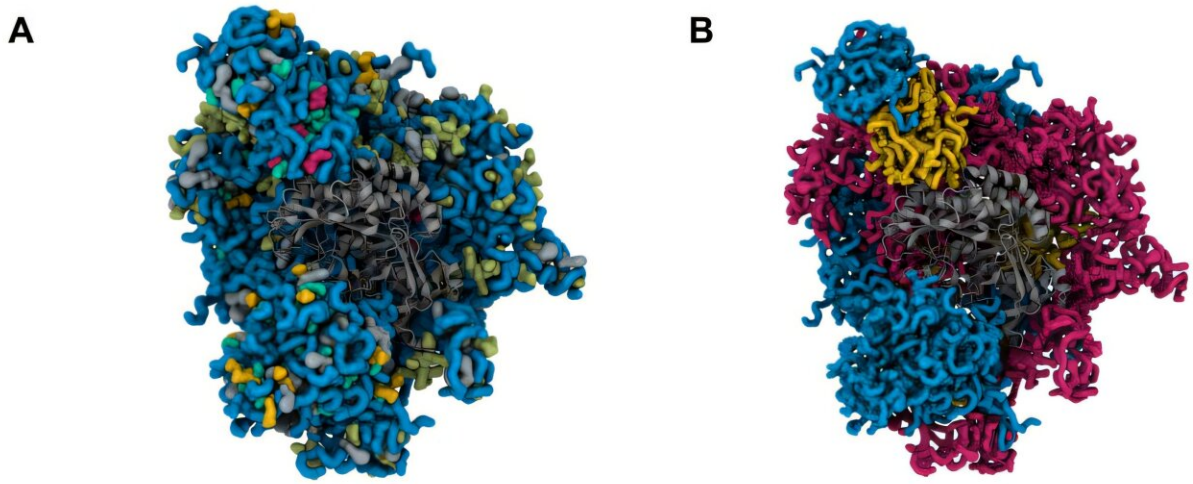

A) Sample snapshot of the simulation demonstrating the possible interaction between the different monomers and GOx at 380K.(B) Sample snapshot of simulation for 10 polymer chains and 1 GOx, demonstrating the possible interaction between the RHPB and GOx. Credit: *ChemRxiv*. 2024; doi:10.26434/chemrxiv-2024-nh0xn

Scientists often seek new materials derived from polymers. Rather than starting a polymer search from scratch, they save time and money by blending existing polymers to achieve desired properties.

But identifying the best blend is a thorny problem. Not only is there a practically limitless number of potential combinations, but polymers interact in complex ways, so the properties of a new blend are challenging to predict.

To accelerate the discovery of new materials, MIT researchers developed a fully autonomous experimental platform that can efficiently identify optimal polymer blends. The paper is published in the journal *Matter*.

The closed-loop workflow uses a powerful algorithm to explore a wide range of potential polymer blends, feeding a selection of combinations to a robotic system that mixes chemicals and tests each blend.

Based on the results, the algorithm decides which experiments to conduct next, continuing the process until the new polymer meets the user's goals.

During experiments, the system autonomously identified hundreds of blends that outperformed their constituent polymers. Interestingly, the researchers found that the best-performing blends did not necessarily use the best individual components.

"I found that to be good confirmation of the value of using an optimization algorithm that considers the full design space at the same time," says Connor Coley, the Class of 1957 Career Development Assistant Professor in the MIT departments of Chemical Engineering and Electrical Engineering and Computer Science, and senior author of the paper.

"If you consider the full formulation space, you can potentially find new or better properties. Using a different approach, you could easily overlook the underperforming components that happen to be the

important parts of the best blend."

This workflow could someday facilitate the discovery of polymer blend materials that lead to advancements like improved battery electrolytes, more cost-effective solar panels, or tailored nanoparticles for safer drug delivery.

Coley is joined on the paper by lead author Guangqi Wu, a former MIT postdoc who is now a Marie Skłodowska-Curie Postdoctoral Fellow at Oxford University; Tianyi Jin, an MIT graduate student; and Alfredo Alexander-Katz, the Michael and Sonja Koerner Professor in the MIT Department of Materials Science and Engineering.

Building better blends

When scientists design new polymer blends, they are faced with a nearly endless number of possible polymers to start with. Once they select a few to mix, they still must choose the composition of each polymer and the concentration of polymers in the blend.

"Having that large of a design space necessitates algorithmic solutions and higher-throughput workflows because you simply couldn't test all the combinations using brute force," Coley adds.

While researchers have studied autonomous workflows for single polymers, less work has focused on polymer blends because of the dramatically larger design space.

In this study, the MIT researchers sought new random heteropolymer blends, made by mixing two or more polymers with different structural features. These versatile polymers have shown particularly promising relevance to high-temperature enzymatic catalysis, a process that increases the rate of chemical reactions.

Their closed-loop workflow begins with an algorithm that, based on the user's desired properties, autonomously identifies a handful of promising polymer blends.

The researchers originally tried a machine-learning model to predict the performance of new blends, but it was difficult to make accurate predictions across the astronomically large space of possibilities. Instead, they utilized a genetic algorithm, which uses biologically inspired operations like selection and mutation to find an optimal solution.

Their system encodes the composition of a polymer blend into what is effectively a digital chromosome, which the genetic algorithm iteratively improves to identify the most promising combinations.

"This algorithm is not new, but we had to modify the algorithm to fit into our system. For instance, we had to limit the number of polymers that could be in one material to make discovery more efficient," Wu adds.

In addition, because the search space is so large, they tuned the algorithm to balance its choice of exploration (searching for random polymers) versus exploitation (optimizing the best polymers from the last experiment).

The algorithm sends 96 polymer blends at a time to the autonomous robotic platform, which mixes the chemicals and measures the properties of each.

The experiments were focused on improving the thermal stability of enzymes by optimizing the retained enzymatic activity (REA), a measure of how stable an enzyme is after mixing with the polymer blends and being exposed to high temperatures.

These results are sent back to the algorithm, which uses them to generate a new set of polymers until the system finds the optimal blend.

Accelerating discovery

Building the robotic system involved numerous challenges, such as developing a technique to evenly heat polymers and optimizing the speed at which the pipette tip moves up and down.

"In autonomous discovery platforms, we emphasize algorithmic innovations, but there are many detailed and subtle aspects of the procedure you have to validate before you can trust the information coming out of it," Coley says.

When tested, the optimal blends their system identified often outperformed the polymers that formed them. The best overall blend performed 18% better than any of its individual components, achieving an REA of 73%.

"This indicates that, instead of developing new polymers, we could sometimes blend existing polymers to design new materials that perform even better than individual polymers do," Wu says.

Moreover, their autonomous platform can generate and test 700 new polymer blends per day and only requires human intervention for refilling and replacing chemicals.

While this research focused on polymers for protein stabilization, their platform could be modified for other uses, like the development of new plastics or battery electrolytes.

In addition to exploring additional polymer properties, the researchers want to use experimental data to improve the efficiency of their

algorithm and develop new algorithms to streamline the operations of the autonomous liquid handler.

More information: Autonomous Discovery of Functional Random Heteropolymer Blends through Evolutionary Formulation Optimization, *Matter* (2025). DOI: 10.1016/j.matt.2025.102336. www.cell.com/matter/fulltext/S2590-2385(25)00379-0 . On *ChemRxiv* DOI: 10.26434/chemrxiv-2024-nh0xn

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