Revolutionizing Material Science with Machine Learning Designed Thermally Robust Shape Memory Vitrimers

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Award Title:	RII Track -1: Louisiana Materials Design Alliance (LAMDA)
NSF Award Number:	NSF OIA-1946231
Principal Investigator:	Michael Khonsari
Lead Institution Name:	Louisiana State University
Award Start Date:	August 1, 2020
Award End Date:	June 30, 2025
Highlight Submission Date:	February 28, 2024

What is the outcome or accomplishment? (1-2 short sentences describing it and why it is transformative; 50-word maximum suggested)*

The study introduces a novel framework (see Fig.1) using machine learning (ML) for designing thermally robust shape memory vitrimers (TRSMVs). This innovative framework successfully overcomes the inherent conflict between molecular chain mobility and the formation and reaction of dynamic covalent bond exchange in vitrimers. Employing this framework, the researchers identified four new types of TRSMVs, with one experimentally validated to exhibit a high glass transition temperature (233.5 °C), impressive recycling efficiency (81.4%), and robust recovery stress (35 MPa).

What is the impact? (1-2 simple sentences describing the benefits for science, industry, society, the economy, national security, *etc.*; suggested 50-word maximum)

This research marks a significant advancement in the field of material science, particularly in the development of shape memory polymers. The successful integration of machine learning approaches into the material design process not only accelerates the discovery of new materials but also enhances the ability to tailor their properties for specific applications. The new TRSMVs designed in this study, exhibiting high thermal robustness, excellent self-healing capacity and efficient shape memory capabilities, are poised to greatly expand the application scope of vitrimers, particularly in demanding environments such as space exploration and high-temperature industrial processes.

What explanation/background does the lay reader need to understand the significance of this outcome? (1-2 paragraphs that might include, for example, more on who, when, where; NSF's role; support from multiple directorates/offices; what makes this accomplishment unique; additional intellectual merits; or broader impacts such as education, outreach, or infrastructure improvement that are integral to this outcome; suggested 150-word maximum)

Shape memory polymers (SMPs) are advanced materials that can return to their original shape when exposed to a specific stimulus, like heat. vitrimers, a subclass of SMPs, are unique because they feature reversible bonds that allow for reshaping and recycling without losing their mechanical strength. However, developing SMPs that maintain both high shape recovery efficiency and high thermal stability has been a longstanding challenge due to the complex interplay of molecular dynamics and bond formation. This study represents a groundbreaking approach using machine learning to design new types of vitrimers that offer both high thermal resistance and efficient recovery, thereby opening up new possibilities for their application in extreme environments and advanced technologies. The research leverages advanced computational models to predict and validate the properties of these new materials, significantly reducing the time and resources needed for traditional trial-and-error experimentation in material science.

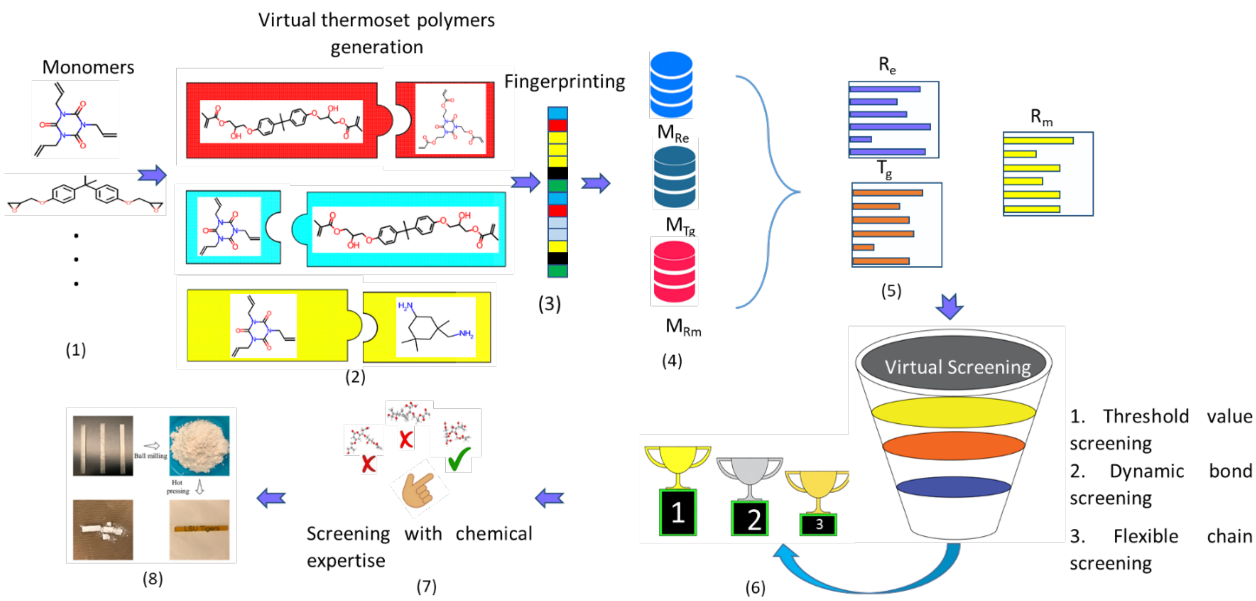

Fig.1 Framework to discover TRSMV: (a) Forward prediction and (b) Inverse mining.