

AI-assisted design of functional polymers for a sustainable world

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Artificial intelligence (AI)-based methods and computational materials science continue to make inroads into accelerated materials design and development. Here, I will review AI-enabled advances made in the subfield of polymer informatics, with a particular focus on the design of application-specific practical polymeric materials. I will describe exemplar design attempts within a few critical and emerging application spaces, including materials designs for storing, producing, and conserving energy, and those that can prepare us for a sustainable economy powered by recyclable and/or biodegradable polymers. AI-powered workflows help efficiently search the staggeringly large chemical and configurational space of materials, using modern machine-learning (ML) algorithms to solve “forward” and “inverse” materials design problems. A theme explored throughout will be a practical informatics-based design protocol that involves creating a set of application-specific target property criteria, building ML model predictors for those relevant target properties, enumerating or generating a tangible population of viable polymers, and selecting candidates that meet design recommendations. The protocol will be demonstrated for several energy and sustainability-related applications. Finally, I will offer an outlook on the lingering obstacles that must be overcome to achieve widespread adoption of informatics-driven protocols in industrial-scale materials development.

References

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