Accelerating Discovery of Sustainable Crosslinked Biopolymers: A Hybrid Supervised and Unsupervised Machine Learning Pipeline for Property Prediction and Performance Mapping for Application-Specific Design

Rajesh, Aswath (School: Viera High School)

This year's engineering project targeted to expand the BioRegen prototype, a waste-derived plastic-alternative optimized for natural biodegradation and performance. The development of a prototype derived from waste materials ensures the construction of a circular economy (an economic model focused on employing all waste to the making of new materials) and the reduction of pollution caused by waste. In order to enhance material performance, three crosslinking agents were incorporated into the polymer prototype—citric, tannic and ferulic acids. Additionally, a plethora of predictive models were included to create a system where a specific bioplastic formulation optimized to fit the user's needs can be easily identified. With the addition of crosslinking agents to the polymer design, significant property improvements were achieved. Specifically, a 67.0% increase in moisture barrier performance, an up to 36.9% increase in tensile strength and a water resistance increase by up to 5.45% was achieved. In addition to mechanical property increases, the environmental safety of the bioplastic was confirmed as 100% of aquatic plants survived after being planted in water where biopolymer had degraded in and a 96% germination rate was achieved in plants planted in soil where BioRegen had biodegraded in. The success in developing a model which incorporates closed-loop valorization demonstrates that, when paired with machine learning, sustainable, high performance bioplastics can be engineered. In addition, the process of closed-loop valorization ensures that waste is diverted from landfills and oceans to the development of usable materials. The involvement of machine learning accelerates the adoption of application-specific products.

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