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AI-Guided Physics-Based Surrogates for Developing Industrial-Grade Bio-Based Elastomers

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Abstract

Developing bio-based elastomers with industrial-grade performance is hindered by the complex chemistry of renewable feedstocks and the high experimental cost of formulation. Lignin-derived polymer systems are particularly attractive, yet difficult to optimize due to their structural variability. Here, we introduce an AI-guided digital formulation twin that accelerates the design of bio-based elastomers by coupling chemistry, processing, mechanics, and sustainability in a single framework. The model integrates polymer descriptors (functionality, oxidation index, polydispersity), process variables, and copolymer composition. Machine-learning models combined with Bayesian multi-objective optimization identify optimal trade-offs between key performance indicators such as storage modulus across 0-60 °C, controlled dissipation, fatigue resistance, and permeability while explicitly enforcing processability and cost constraints. To strengthen predictive capability, we implement a physics-based machine-learning (PBML) strategy. Experimental data from targeted mechanical tests on fabricated elastomers where tensile, compressive, dynamic, and others responses will be fused with constitutive models to train algorithms that learn the links between molecular structure, processing parameters, and mechanical behavior. The resulting surrogates progressively reduce the need for physical testing and deliver finite-element-ready

parameters for virtual component validation. The framework operates in adaptive design build-test-learn cycles with uncertainty quantification and SHAP-based explainability to prioritize promising chemistries and processing windows. Validation combines rheology, DMA, and fatigue testing with functional trials in technical seals and flexible protective components. The methodology is coupled in-line with life-cycle assessment (LCA) and techno-economic assessment (TEA) to co-optimize performance, cost, and carbon footprint, demonstrating significant impact reductions and industrial scalability. Overall, this approach establishes a transferable route for AI-guided, physics-informed, sustainable formulation of high-performance bio-based elastomers.

Keywords:

Physics-based machine learning Bayesian multi-objective optimization Digital formulation twin Lignin-based elastomers Mechanical performance prediction FEM-ready parameters LCA/TEA Design-build-test-learn cycles Sustainable materials design