Active machine learning for new monomers for frontal ring-opening metathesis polymerization

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Thermoset polymers and composites are widely used in airplanes, cars, and structural components due to their strength, stiffness, and low density. However, traditional thermosets require large amounts of energy to cure. Frontal ring-opening metathesis polymerization (FROMP) only requires a small initial thermal or photo stimulus which triggers a self-propagating exothermic reaction that fully cures the monomer to polymer. Currently, there are only a small number of monomers that can sustain FROMP. We use active machine learning (ML) to identify new FROMP-able monomers. The active learning cycle uses an ML model of the small pool of currently known FROMP monomers, then predicts outcomes across a database of candidate monomers, and identifies the candidate monomer that will most improve the model's predictions. The chosen monomer is synthesized and tested before feeding the resulting information back to the model. This process was repeated until the pool of FROMP-suitable monomers is expanded, and the uncertainty of the predictions is sufficiently low. We will also use all the data generated to build a classification ML model. This model can identify key features that determine whether a monomer is FROMP-able. This research has expanded the pool of FROMP-suitable monomers and will develop guidelines for future FROMP monomer development.