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(54) Title: MOLECULAR GRAPH STRUCTURE BASED MODELING TO PREDICT PROPERTIES OF POLYMERS UTILIZING LOCAL CLUSTERS

(57) Abstract: In at least one example, a method for molecular graph structure based modeling to predict properties of polymers utilizing local cluster includes generating a data set that includes a respective structure and properties for each of a plurality of monomers corresponding to a designated polymer, converting the respective structures to graph connectivity structures, determining a plurality of local clusters based on the plurality of monomers, calculating a respective polymeric property of each of the plurality of local clusters based on density functional theory (DFT), inputting monomer data to a machine learning model trained to determine an unknown polymeric property of a designated polymer from an output value of a graph neural network and the respective polymeric properties for a plurality of identified local clusters from the designated polymer, and receiving a prediction of the unknown polymeric property of the designated polymer from the machine learning model.