

# Prediction and Interpretation of Polymer Properties Using the Graph Convolutional Network

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**ABSTRACT:** We present machine learning models for the prediction of thermal and mechanical properties of polymers based on the graph convolutional network (GCN). GCN-based models provide reliable prediction performances for the glass transition temperature ( $T_g$ ), melting temperature ( $T_m$ ), density ( $\rho$ ), and elastic modulus ( $E$ ) with substantial dependence on the dataset, which is the best for  $T_g$  ( $R^2 \sim 0.9$ ) and worst for  $E$  ( $R^2 \sim 0.5$ ). It is found that the GCN representations for polymers provide prediction performances of their properties comparable to the popular extended-connectivity circular fingerprint (ECFP) representation. Notably, the GCN combined with the neural network regression (GCN-NN) slightly outperforms the ECFP. It is investigated how the GCN captures important structural features of polymers to learn their properties. Using the dimensionality reduction, we demonstrate that the polymers are organized in the principal subspace of the GCN representation spaces with respect to the backbone rigidity. The organization in the representation space adaptively changes with the training and through the NN layers, which might facilitate a subsequent prediction of target properties based on the relationships between the structure and the property. The GCN models are found to provide an advantage to automatically extract a backbone rigidity, strongly correlated with  $T_g$ , as well as a potential transferability to predict other properties associated with a backbone rigidity. Our results indicate both the capability and limitations of the GCN in learning to describe polymer systems depending on the property.

**KEYWORDS:** machine learning, graph convolutional network, molecular featurization, backbone rigidity, polymer property prediction, neural network



## 1. INTRODUCTION

Machine learning (ML) has been influencing many facets of materials sciences and chemistry by providing powerful techniques of leveraging data, which enables rapid prediction of properties, the discovery of novel molecules, and the route of synthesis.<sup>1–3</sup> An application of ML to polymer systems is promising because they exhibit interesting physical phenomena over extensive time and length scales in none-equilibrium glassy states for which experimental characterization and simulations are relatively costly and difficult.<sup>4–6</sup> This indicates also the challenges in the application of ML because the power of ML hinges on a high-quality database.<sup>7</sup> The promise of ML triggered a surge of studies on polymers to predict a range of physical properties with various learning algorithms,<sup>8–10</sup> to build a database of the prediction models,<sup>11</sup> and to augment the polymer structure database.<sup>12</sup> Also, the transfer learning and generative model were combined to overcome the problem of limited data such as thermal conductivity and to discover the novel polymers.<sup>13</sup>

ML models learn the complex patterns in data through the suitable representation of the data.<sup>14</sup> The conventional

molecular representation is a list of features hand-crafted based on domain knowledge for the quantitative structure–activity relationships.<sup>15</sup> On the other hand, extended-connectivity circular fingerprints (ECFPs) are widely used methods that exploit the graph structures of molecules to encode the presence of particular substructures of chosen scale into discrete bit vector representations.<sup>16</sup> Deep learning-based approaches like the graph convolutional network (GCN) are the state-of-the-art learning method for graph-structured data and can be used to generate representations of molecules.<sup>17</sup> The GCN-based representation is promising compared to the hand-crafted descriptors or the ECFP representations because it can be optimized for data domains through the supervision.<sup>17</sup> Also, the GCN generates continuous representations

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# Prediction Of Polymer Properties

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Fried, 2014-07-01 The Definitive Guide to Polymer Principles Properties Synthesis Applications and Simulations Now fully revised Polymer Science and Technology Third Edition systematically reviews the field's current state and emerging advances Leading polymer specialist Joel R Fried offers modern coverage of both processing principles and applications in multiple industries including medicine biotechnology chemicals and electronics This edition's new and expanded coverage ranges from advanced synthesis to the latest drug delivery applications New topics include controlled radical polymerization click chemistry green chemistry block copolymers nanofillers electrospinning and more A brand new chapter offers extensive guidance for predicting polymer properties including additional coverage of group correlations and new discussions of the use of topological indices and neural networks This is also the first introductory polymer text to fully explain computational polymer science including molecular dynamics and Monte Carlo methods Simulation concepts are supported with many application examples ranging from prediction of PVT values to permeability and free volume Fried thoroughly covers synthetic polymer chemistry polymer properties in solution and in melt rubber and solid states and all important categories of plastics This revised edition also adds many new calculations end of chapter problems and references In depth coverage includes Polymer synthesis step and chain growth bulk solution suspension emulsion solid state and plasma ionic liquids and macromers and genetic engineering Amorphous and crystalline states transitions mechanical properties and solid state characterization Polymers and the environment degradation stability and more Additives blends block copolymers and composites including interpenetrating networks nanocomposites buckyballs carbon nanotubes graphene and POSS Biopolymers natural polymers fibers thermoplastics elastomers and thermosets Engineering and specialty polymers from polycarbonates to ionic polymers and high performance fibers Polymer rheology processing and modeling Correlations and simulations group contribution topological indices artificial neural networks molecular dynamics and Monte Carlo simulations Joint Conference of Italian, Austrian, Slovenian Rheologists RHEOtech, Gruppo italiano di reologia, 1998

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Properties of Polymers D.W. van Krevelen, Klaas te Nijenhuis, 2009-02-09 This authoritative widely cited book has been used all over the world Properties of Polymers Fourth Edition incorporates the latest developments in the field while

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