

Prediction and Interpretation of Polymer Properties Using the Graph Convolutional Network

Jachong Park, Youngseon Shim,* Franklin Lee, Aravind Rammohan, Sushmit Goyal, Munbo Shim, Changwook Jeong,* and Dae Sin Kim



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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 (ρ), 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.^{1–3} 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.^{4–6} This indicates also the challenges in the application of ML because the power of ML hinges on a high-quality database.⁷ The promise of ML triggered a surge of studies on polymers to predict a range of physical properties with various learning algorithms,^{8,9} to build a database of the prediction models,¹⁰ and to augment the polymer structure database.¹¹ 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.¹²

ML models learn the complex patterns in data through the suitable representation of the data.¹³ The conventional



molecular representation is a list of features hand-crafted based on domain knowledge for the quantitative structure–activity relationships.¹⁴ 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.¹⁵ 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.¹⁶ 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.¹⁷ Also, the GCN generates continuous representations

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Prediction Of Polymer Properties

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Table of Contents Prediction Of Polymer Properties

1. Understanding the eBook Prediction Of Polymer Properties
 - The Rise of Digital Reading Prediction Of Polymer Properties
 - Advantages of eBooks Over Traditional Books
2. Identifying Prediction Of Polymer Properties
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Prediction Of Polymer Properties
 - User-Friendly Interface
4. Exploring eBook Recommendations from Prediction Of Polymer Properties
 - Personalized Recommendations
 - Prediction Of Polymer Properties User Reviews and Ratings
 - Prediction Of Polymer Properties and Bestseller Lists
5. Accessing Prediction Of Polymer Properties Free and Paid eBooks

- Prediction Of Polymer Properties Public Domain eBooks
- Prediction Of Polymer Properties eBook Subscription Services
- Prediction Of Polymer Properties Budget-Friendly Options
- 6. Navigating Prediction Of Polymer Properties eBook Formats
 - ePub, PDF, MOBI, and More
 - Prediction Of Polymer Properties Compatibility with Devices
 - Prediction Of Polymer Properties Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Prediction Of Polymer Properties
 - Highlighting and Note-Taking Prediction Of Polymer Properties
 - Interactive Elements Prediction Of Polymer Properties
- 8. Staying Engaged with Prediction Of Polymer Properties
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Prediction Of Polymer Properties
- 9. Balancing eBooks and Physical Books Prediction Of Polymer Properties
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Prediction Of Polymer Properties
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Prediction Of Polymer Properties
 - Setting Reading Goals Prediction Of Polymer Properties
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Prediction Of Polymer Properties
 - Fact-Checking eBook Content of Prediction Of Polymer Properties
 - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development

- Exploring Educational eBooks

14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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