

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 (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

Vassilios Galiatsatos



Prediction Of Polymer Properties:

Prediction of Polymer Properties Jozef Bicerano, 2002-08-01 Highlighting a broad range multiscale modeling and methods for anticipating the morphologies and the properties of interfaces and multiphase materials this reference covers the methodology of predicting polymer properties and its potential application to a wider variety of polymer types than previously thought possible A comprehensive source the **Novel Computational Techniques for the Prediction of Polymer Properties** B. Jeffrey Sherman, 1998 **Modification of Polymer Properties** Carlos Federico Jasso-Gastinel, José M. Kenny, 2016-09-14 Modification of Polymer Properties provides for the first time in one title the latest information on gradient IPNs and gradient copolymers The book covers the broad range of polymer modification routes in a fresh current view representing a timely addition to the technical literature of this important area Historically blends copolymers or filled polymers have been developed to meet specific properties or to optimize the cost properties relationship Using the gradient structure approach with conventional radical polymerization it has been shown that it is possible to optimize properties if appropriate gradients in the composition of copolymer chains are obtained An overview of the gradient structure approach for designing polymers has not appeared in the recent literature and this title covers the different methods used to modify properties offering the whole range of ways to modify polymers in just one volume and making this an attractive option for a wide audience of practitioners The approach for each chapter is to explain the fundamental principles of preparation cover properties modification describe future research and applications as examples of materials that may be prepared for specific applications or that are already in use in present day applications The book is for readers that have a basic background in polymer science as well as those interested in the different ways to combine or modify polymer properties Provides an integrated view on how to modify polymer properties Presents the entire panorama of polymer properties modification in one reference covering the essential information in each topic Includes the optimization of properties using gradients in polymers composition or structure Multiscale Modelling of Polymer Properties E. Perpète, Manuel Laso, 2006-11-18 Modelling in polymer materials science has experienced a dramatic growth in the last two decades Advances in modeling methodologies together with rapid growth in computational power have made it possible to address increasingly complex questions both of a fundamental and of a more applied nature Multiscale Modelling of Polymer Properties assembles research done on modeling of polymeric materials from a hierarchical point of view in which several methods are combined in a multilevel approach to complex polymeric materials Contributions from academic and industrial experts are organized in two parts the first one addresses the methodological aspects while the second one focuses on specific applications The book aims at comprehensively assessing the current state of the field including the strengths and shortcomings of available modelling techniques and at identifying future needs and trends Several levels of approximation to the field of polymer modelling ranging from first principles to purely macroscopic Contributions from both academic and industrial experts with varying

fields of expertise Assesses current state of this emerging and rapidly growing field *Molecular Simulation Methods for Predicting Polymer Properties* Vassilios Galiatsatos, 2005-02-03 Among the thousands of synthesized polymers new polymeric substances and materials with new often unusual properties often arise Consequently this presents a problem in determining the physical properties of polymers and thus makes it difficult to ascertain how to synthesize polymers with desired properties This book discusses what molecular modelling can do to predict the properties of realistic polymer systems Organized by property each chapter will address the methods one may use to study the particular system Focuses on polymer properties rather than methods making it more accessible to the average scientist engineer All important polymers will be covered such as amorphous polymers semicrystalline polymers elastomers emulsions polymer interfaces and surfaces Chapters contributed by experts in the field Discusses current commercial software used in molecular simulation

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