

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,^{8–10} to build a database of the prediction models,¹¹ and to augment the polymer structure database.¹² 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.¹³

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



molecular representation is a list of features hand-crafted based on domain knowledge for the quantitative structure–activity relationships.¹⁵ 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.¹⁶ 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.¹⁷ 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

**Leonard Barolli, Nadeem Javaid, Makoto
Ikeda, Makoto Takizawa**



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

Polymer Properties Prediction Programs Wendell W. Catron, 1988 **Predicting Polymer Properties by Computational Methods 2**, 1992 Polymer Science and Technology Joel R. Fried, 2014 This text describes how plastics rubber and fibers are synthesized processed into useful materials characterized and compounded with fillers and other additives to improve performance for specific applications Their use in a wide variety of technologies including membrane separations electronics and energy production and storage is described A new chapter in the Third Edition shows how computer correlations and simulations can be used to predict properties of new plastics and to better understand how existing plastics perform **Modelling of Chemical Reaction Systems** K.H. Ebert, P. Deuflhard, W. Jäger, 2012-12-06 For rather a long time numerical results in chemical kinetics could only be obtained for very simple chemical reactions most of which were of minor practical importance The availability of fast computers has provided new opportunities for developments in chemical kinetics Chemical systems of practical interest are usually very complicated They consist of a great number of different elementary chemical reactions mostly with rate constants differing by many orders of magnitude frequently with surface reaction steps and often with transport processes The derivation of a true chemical mechanism can be extremely cumbersome Mostly this work is done by setting up reaction models which are improved step by step in comparison with precise experimental data At this early stage mathematics is involved which may already be rather complicated Mathematical methods such as perturbation theory graph theory sensitivity analysis or numerical integration are necessary for the derivation and application of optimal chemical reaction models Most theoretical work aimed at improving the mathematical methods was done on chemical reactions which mostly were of little practical importance Chemical engineers who evidently know well how important the chemical models and their dynamics are for reactor design have also to be convinced not only on the theoretical work but also on its practical applicability **Machine Learning for Polymer Informatics** Ying Li, Tianle Yue, 2024-06-28 Machine learning has significantly accelerated the development of new polymer materials Machine Learning for Polymer Informatics introduces the reader to the most popular ways of applying machine

learning in polymer informatics This primer will equip the reader to ask the right questions about the application of machine learning in their areas of interest as well as critically interpret publications leveraging machine learning methods The authors encourage readers to try machine learning techniques when they have sufficient data in their area of interest The development of machine learning has far exceeded human imagination and with sufficient data everything is full of possibilities

Polymer Surface Characterization Luigia Sabbatini, Elvira De Giglio, 2022-01-19 This fully updated edition provides a broad approach to the surface analysis of polymers being of high technological interest Modern analytical techniques potential applications and recent advances in instrumental apparatus are discussed The self consistent chapters are devoted to spectroscopic and microscopic techniques which represent powerful tools for the characterization of morphology and chemical physical mechanical properties of polymer surfaces interfaces and thin films Selection of techniques which can properly address very shallow depth of surfaces spanning from few angstroms to tens of nanometers Interaction of polymer surfaces with their surroundings is pointed out as a critical issue for specific applications

Quantitative Predictions of Polymer Melt Dynamics Cattaleeya Pattamaprom, 2001 **Materials Informatics III** Kunal Roy, Arkaprava Banerjee, 2025-03-01 This contributed volume focuses on the application of machine learning and cheminformatics in predictive modeling for organic materials polymers solvents and energetic materials It provides an in depth look at how machine learning is utilized to predict key properties of polymers deep eutectic solvents and ionic liquids as well as to improve safety and performance in the study of energetic and reactive materials With chapters covering polymer informatics quantitative structure property relationship QSPR modeling and computational approaches the book serves as a comprehensive resource for researchers applying predictive modeling techniques to advance materials science and improve material safety and performance *Advances in Engineering Materials* Tamara Tatishvili, A. K.

Haghi, 2025-07-11 This new book covers the most recent developments in materials technology and science providing deep insight into advanced materials in regard to structural and physical behavior and sustainable real world applications It discusses the practical applications of novel materials for emerging technologies highlighting interesting and exciting mechanical and chemical behaviors and properties of new materials The volume also addresses the relationship between structural identities of materials with their property profile It explains the way we control the process parameters during the preparation of materials in detail in order to obtain the desired features in the form of arrangement of atoms ions or molecules and thereby the preparation of the materials to be in line with real world applications **Characterisation of Copolymers**, 1995

Handbook of Polymer Synthesis, Characterization, and Processing Enrique Saldivar-Guerra, Eduardo Vivaldo-Lima, 2013-02-28 Covering a broad range of polymer science topics Handbook of Polymer Synthesis Characterization and Processing provides polymer industry professionals and researchers in polymer science and technology with a single comprehensive handbook summarizing all aspects involved in the polymer production chain The handbook focuses on

industrially important polymers analytical techniques and formulation methods with chapters covering step growth radical and co polymerization crosslinking and grafting reaction engineering advanced technology applications including conjugated dendritic and nanomaterial polymers and emulsions and characterization methods including spectroscopy light scattering and microscopy

17th European Symposium on Computed Aided Process Engineering Valentin Plesu, Paul Serban Agachi, 2007-05-24 The 17th European Symposium on Computed Aided Process Engineering contains papers presented at the 17th European Symposium of Computer Aided Process Engineering ESCAPE 17 held in Bucharest Romania from 27-30 May 2007 The ESCAPE series serves as a forum for scientists and engineers from academia and industry to discuss progress achieved in the area of Computer Aided Process Engineering CAPE The main goal was to emphasize the continuity in research of innovative concepts and systematic design methods as well the diversity of applications emerged from the demands of sustainable development ESCAPE 17 highlights the progress software technology needed for implementing simulation based tools The symposium is based on 5 themes and 27 topics following the main trends in CAPE area Modelling Process and Products Design Optimisation and Optimal Control and Operation System Biology and Biological Processes Process Integration and Sustainable Development Participants from 50 countries attended and invited speakers presented 5 plenary lectures tackling broad subjects and 10 keynote lectures Satellite events added a plus to the scientific dimension to this symposium All contributions are included on the CD ROM attached to the book Attendance from 50 countries with invited speakers presenting 5 plenary lectures tackling broad subjects and 10 keynote lectures

Forcefields for Atomistic-Scale Simulations: Materials and Applications Akarsh Verma, Sanjay Mavinkere Rangappa, Shigenobu Ogata, Suchart Siengchin, 2022-08-19 This book describes the forcefields interatomic potentials that are used in the atomistic scale and molecular dynamics simulations It covers mechanisms salient features formulations important aspects and case studies of various forcefields utilized for characterizing various materials such as nuclear materials and nanomaterials and applications This book gives many help to students and researchers who are studying the forcefield potentials and introduces various applications of atomistic scale simulations to professors who are researching molecular dynamics

Complex, Intelligent, and Software Intensive Systems Leonard Barolli, Nadeem Javaid, Makoto Ikeda, Makoto Takizawa, 2018-06-18 This book provides a platform of scientific interaction between the three challenging and closely linked areas of ICT enabled application research and development software intensive systems complex systems and intelligent systems Software intensive systems strongly interact with other systems sensors actuators devices other software systems and users More and more domains are using software intensive systems e.g. automotive and telecommunication systems embedded systems in general industrial automation systems and business applications Moreover web services offer a new platform for enabling software intensive systems Complex systems research is focused on the overall understanding of systems rather than their components Complex systems are characterized by the changing environments in which they interact They evolve and adapt

through internal and external dynamic interactions The development of intelligent systems and agents which are increasingly characterized by their use of ontologies and their logical foundations offer impulses for both software intensive systems and complex systems Recent research in the field of intelligent systems robotics neuroscience artificial intelligence and cognitive sciences are vital for the future development and innovation of software intensive and complex systems **Advanced Topics in Polymer Chemistry and Materials Science** Tamara Tatrishvili, Marc Jean Médard Abadie, 2025-07-11 Advanced polymers also known as engineering polymers or high performance polymers are synthetic polymers with exceptional mechanical thermal chemical and electrical properties high heat and thermal stability frost resistance hydrophobicity high dielectric indices etc This new volume focuses on a particular applied objective the creation of new polymeric materials with improved properties The volume highlights new concepts achievements and investigations in polymer chemistry and chemical engineering and provides a survey of the important categories of polymers including commodity thermoplastics and fibers elastomers and thermosets and engineering and specialty polymers Scientists and researchers in the field of polymer functional materials will find much food for thought in this volume

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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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