

Feature Article

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Polymer Genome: A Data-Powered Polymer Informatics Platform for Property Predictions

Chiho Kim,^{†,¶} Anand Chandrasekaran,^{†,¶} Tran Doan Huan,[‡] Deya Das,[†] and
Rampi Ramprasad^{*,†}

†School of Materials Science and Engineering, Georgia Institute of Technology, 771 Ferst Dr. NW, Atlanta, GA 30332, USA

‡Department of Materials Science and Engineering and Institute of Materials Science, University of Connecticut, 97 North Eagleville Rd., Storrs, Connecticut 06269-3136, USA

¶Contributed equally to this work

E-mail: rampi.ramprasad@mse.gatech.edu

Abstract

The recent successes of the Materials Genome Initiative has opened up new opportunities for data-centric informatics approaches in several subfields of materials research, including in polymer science and engineering. Polymers, being inexpensive and possessing a broad range of tunable properties, are widespread in many technological applications. The vast chemical and morphological complexity of polymers though gives rise to challenges in the rational discovery of new materials for specific applications. The nascent field of polymer informatics seeks to provide tools and pathways for accelerated property prediction (and materials design) via surrogate machine learning models built on reliable past data. We have carefully accumulated a dataset of organic polymers whose properties were obtained either computationally (bandgap, dielectric constant, refractive index and atomization energy) or experimentally (glass transition temperature, solubility parameter and density). A fingerprinting scheme that captures atomistic to morphological structural features was developed to numerically represent the polymers. Machine learning models were then trained by mapping the fingerprints (or features) to properties. Once developed, these models can rapidly predict properties of new polymers (within the same chemical class as the parent dataset) and can also provide uncertainties underlying the predictions. Since different properties depend on different length-scale features, the prediction models were built on an optimized set of features for each individual property. Furthermore, these models are incorporated in a user friendly online platform named Polymer Genome (www.polymergenome.org). Systematic and progressive expansion of both chemical and property spaces are planned to extend the applicability of Polymer Genome to a wide range of technological domains.

1 1 Introduction

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6 The past few years have seen a surge in the application of data-driven techniques in a plethora
7 of research and development fields, ranging from image-recognition¹ to drug-discovery.^{2,3}
8 Sophisticated machine learning techniques, initially within the purview of computer science
9 researchers mainly, are now becoming ubiquitous in many other branches of science and
10 engineering, and have the potential to spur technological innovations.
11
12

13 In materials science, the increasing availability of large amounts of data (both computa-
14 tional and experimental) has led to the prominent field of materials informatics over the past
15 few years.^{4–21} The strategic visions and plans of the Materials Genome Initiative (USA)²²
16 and the recent developments of essential infrastructures for materials informatics such as the
17 NOMAD Laboratory: a European Centre for Excellence (EU),²³ and the Materials Research
18 by Information Integration Initiative (Japan) are expected to lead to a paradigm shift in the
19 discovery of novel functional materials.²⁴
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22 Polymers form an important (and challenging) materials class. They are pervasive with
23 applications ranging from daily products, e.g., plastic packaging and containers, to state-of-
24 the-art technological components, e.g., high-energy density capacitors, electrolytes for Li-ion
25 batteries, polymer light-emitting diodes, and photovoltaic materials. Their chemical and
26 morphological spaces are immensely vast and complex,²⁵ leading to fundamental obstacles
27 in polymer discovery. Some recent successes in rationally designing polymer dielectrics via
28 experiment-computation synergies^{4,5,13,17,26–33} indicate that there may be opportunities for
29 machine learning and informatics approaches in this challenging research and development
30 area.

31 The biggest hurdle of the machine learning approach to polymer discovery is of both
32 scientific and non-scientific in nature. The properties of a polymer are strongly dependent
33 on distinctive factors such as branching, molecular weight distribution, copolymerization,
34 additives and processing conditions. These factors, along with issues such as non-standard
35 naming conventions, have made it exceedingly difficult to create a universal polymer database
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upon which one may base a polymer informatics framework. A detailed analysis of the challenges faced in this front is presented in a recent review paper by Audus and de Pablo.³⁴

We have created an informatics platform capable of predicting a variety of important polymer properties on-demand. This platform utilizes surrogate (or machine learning) models, which link key features of polymers to properties, trained on high-throughput DFT calculations and experimental data from literature and existing databases. This dataset of 854 polymers and the properties considered thus far are summarized in Figure 1. Certain properties, like the atomization energy, depend mainly on the atomic constituents and short-range bonding, whereas other properties, such as the glass transition temperature (T_g), are strongly influenced by morphological characteristics like the chain-stiffness and branching. We have constructed a hierarchical and automated fingerprinting scheme to identify the most important set of features to accurately describe a particular polymer property. The features span multiple length scales and range from 3-atom long fragments to descriptors such as the ratio of side-chain and main-chain atoms. The description of polymers in terms of these fundamental chemical and morphological “building blocks” is what inspired the coinage of the term “Polymer Genome”. Machine learning algorithms, specifically those based on Gaussian process regression (GPR),³⁵ were used to generate predictive models to correlate the polymer’s ‘genome’ to its associated properties. The property prediction models have been implemented in an online platform (www.polymergenome.org), to guide polymer choices for further investigation via synthesis.

This article is organized as follows. In Sec. 2, we describe the curation of high-throughput computational data for polymers built using a set of predefined chemical “blocks”, and experimental data, which were obtained from existing databases.^{36,37} In Sec. 3, we describe the hierarchy of descriptors used to fingerprint the polymers. In Sec. 4, various aspects of prediction model development, e.g., the fingerprint dimensionality reduction schemes and machine learning algorithms, are described in detail. The predictive accuracy of the model, using the aforementioned hierarchical fingerprinting scheme, is demonstrated for the partic-

ular case of T_g . The performance of the final models for all the properties are summarized in Sec. 5. In Sec. 6, we provide an overview of our online polymer property prediction platform. Details of how this platform may be used (including how polymers may be queried using a customized SMILES string language) are provided separately in the Appendix.

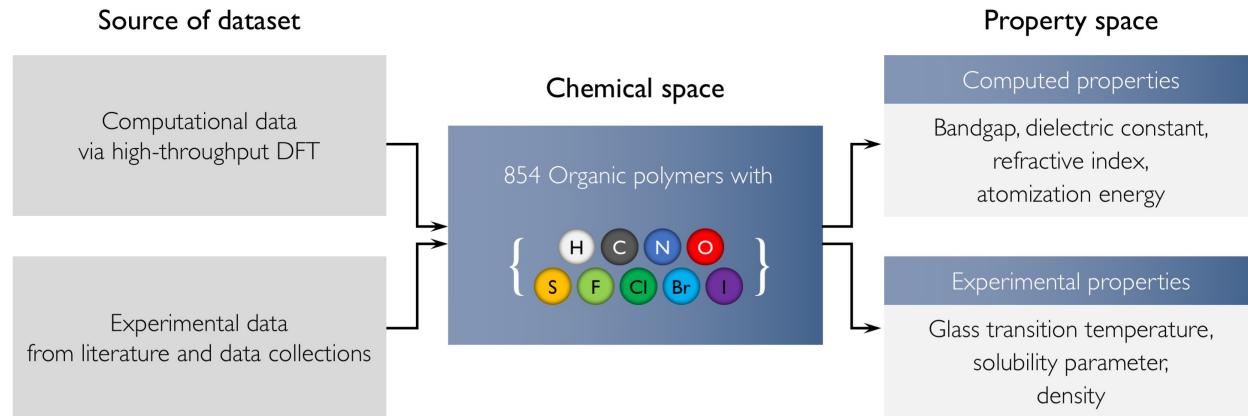


Figure 1: Overview of our polymer dataset used for development of property prediction models.

2 Dataset

Two strategic tracks were followed for the creation of our dataset (see Figure 1): (1) via high-throughput computation using density functional theory (DFT) as presented earlier,^{26,38,39} and (2) by utilizing experimentally measured properties from literature and data collections.^{36,37} The overall dataset includes 854 polymers made up of a subset of the following species: H, C, N, O, S, F, Cl, Br and I. Seven different properties were included in the present study. The bandgap, dielectric constant, refractive index and atomization energy were determined using DFT computations, and T_g , solubility parameter and density were obtained from measurements.

All the computational data was generated through a series of studies related to advanced polymer dielectrics.^{26,38,39} The computational dataset includes polymers containing the following building blocks, CH_2 , CO, CS, NH, C_6H_4 , $\text{C}_4\text{H}_2\text{S}$, CF_2 , CHF and O.^{13,16,38–40} Repeat

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3 units contained 4-8 building blocks, and 3D structure prediction algorithms were used to de-
4 termine their structure.^{26,38,39} The building blocks considered in the dataset are found in com-
5 mon polymeric materials including polyethylene (PE), polyesters and polyureas, and could
6 theoretically produce an enormous variety of different polymers. The bandgap was com-
7 puted using the hybrid Heyd-Scuseria-Ernzerhof (HSE06) electronic exchange-correlation
8 functional.⁴¹ Dielectric constant and refractive index (the square root of the electronic
9 part of the dielectric constant) were computed using density functional perturbation theory
10 (DFPT).⁴² The atomization energy was computed for all the polymers following previous
11 work.^{28-31,39,40,43-48}

12
13 The T_g , solubility parameter and density data was obtained from existing databases of
14 experimental measurements.^{36,37} T_g , which is an indication of the transition point between
15 the glassy and supercooled liquid phases in an amorphous polymer, is important in many
16 polymer applications because the structural characteristics (and, consequently, other prop-
17 erties) of the polymer changes dramatically at this point. The solubility parameter of a
18 polymer is typically used to determine a suitable solvent to use during polymer synthesis. In
19 this particular study we consider the Hildebrand solubility parameter, which is also useful
20 to make quantitative estimation of polymer-solvent interaction.⁴⁹⁻⁵¹

21
22 We have determined the chemical formula and the associated topological structure from
23 the name of polymers listed in the literature. The dataset contains a total of 854 organic
24 polymers composed of 9 frequently found atomic species; i.e, C, H, O, N, S, F, Cl, Br and I
25 with properties listed in the right side panel of Figure 1. Figure 2 shows a summary of the
26 property space for the polymer dataset, including the range of property values, distribution,
27 standard deviation and the number of polymers associated with each property.

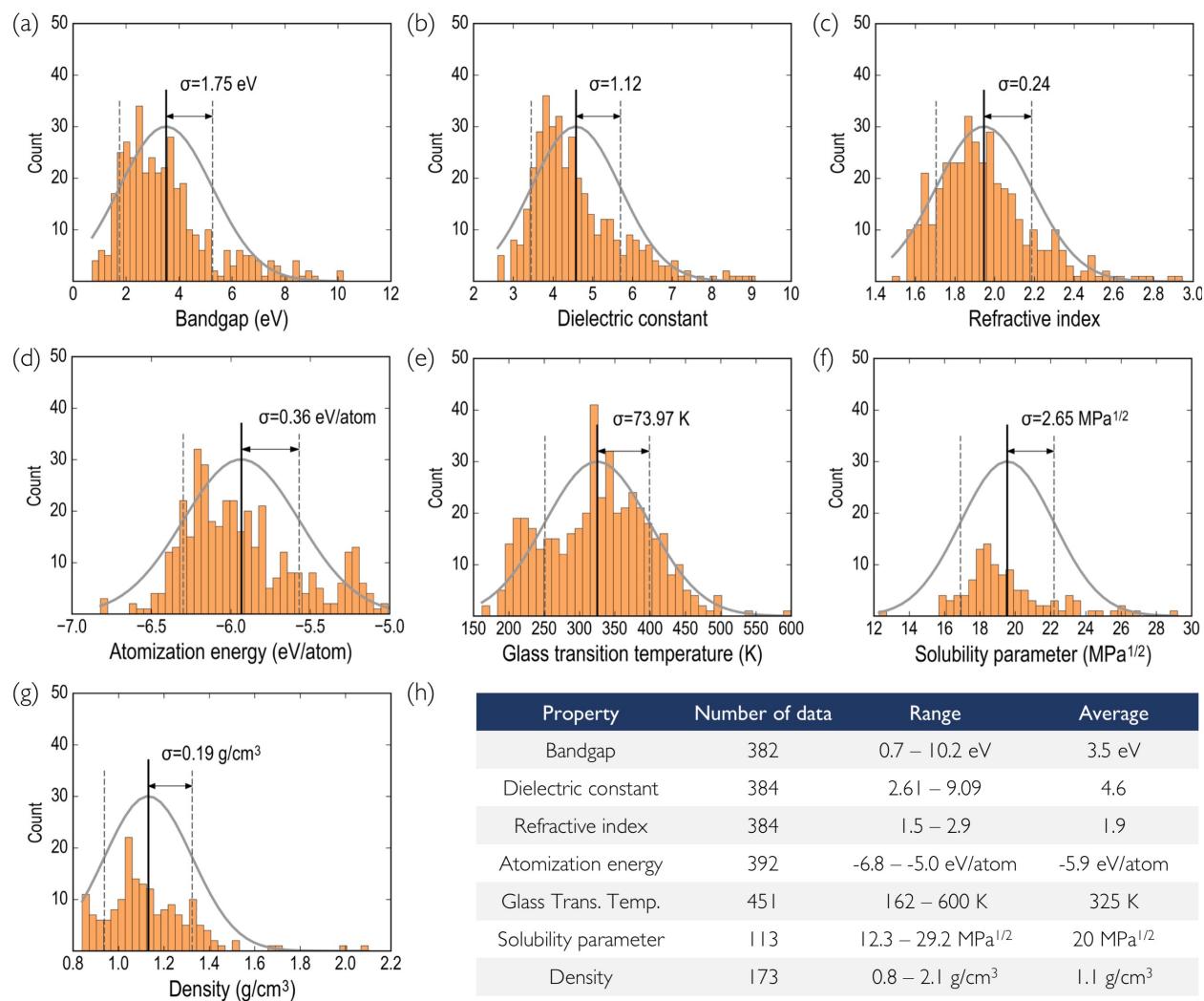


Figure 2: Property space of Polymer Genome dataset. The 7 properties considered in this study were the bandgap, dielectric constant, refractive index, atomization energy, T_g , solubility parameter and density.

3 Hierarchical fingerprinting

Fingerprinting is a crucial step of our data-driven machine learning approach. In this step, the geometric and chemical information of the polymers is converted to a numerical representation. To comprehensively capture the key features that may control the diversity of properties of interest, we consider three hierarchical levels of descriptors spanning different length scales. At the atomic-scale, the occurrence of a fixed set of atomic fragments (or

motifs) are tracked.⁵² An example of such a fragment is 01-C3-C4, made up of three contiguous atoms, namely, a one-fold coordinated oxygen, a three-fold coordinated carbon, and a four-fold coordinated carbon, in this order. Such a series of predefined "triplets" has been shown to be a good fingerprint for a diverse range of organic materials.^{17,52} A vector of such triplets form the fingerprint components at the lowest hierarchy. For the polymer class under study, there are 108 such components.

Next in the hierarchy of fingerprint components are larger length-scale descriptors of the quantitative structure-property relationship (QSPR) type, often used in chemical and biological sciences, and implemented in the RDKit Python library.^{53–55} Examples of such descriptors are van der Waals surface area,⁵⁶ the topological polar surface area (TPSA),^{57,58} the fraction of atoms that are part of rings (i.e., the number of atoms associated with rings divided by the total number of atoms in the formula unit), and the fraction of rotatable bonds. TPSA is the sum of surfaces of polar atoms in the molecule and we observed this descriptor to be strongly correlated to the solubility. Descriptors such as the fraction of ring atoms and fraction of rotatable bonds strongly influenced properties such as T_g and density. Such descriptors, 99 in total, form the next set of components of our overall fingerprint.

The highest length-scale fingerprint components we considered may be classified as "morphological descriptors". These include features such as the shortest topological distance between rings, fraction of atoms that are part of side-chains, and the length of the largest side-chain. Properties such as T_g strongly depend on such features which influence the way the chains are packed in the polymer. For instance, if two rings are very close, the stiffness of the polymer backbone is much higher than if the rings were separated by a larger topological distance. Both the number and the length of the side-chains strongly influence the amount of free volume in the polymeric material and therefore directly influence T_g . The larger the free-volume, the lower the T_g . We include 22 such morphological descriptors in our overall fingerprint.

Figure 3a shows the hierarchy of polymer fingerprint, including atomic level, QSPR and

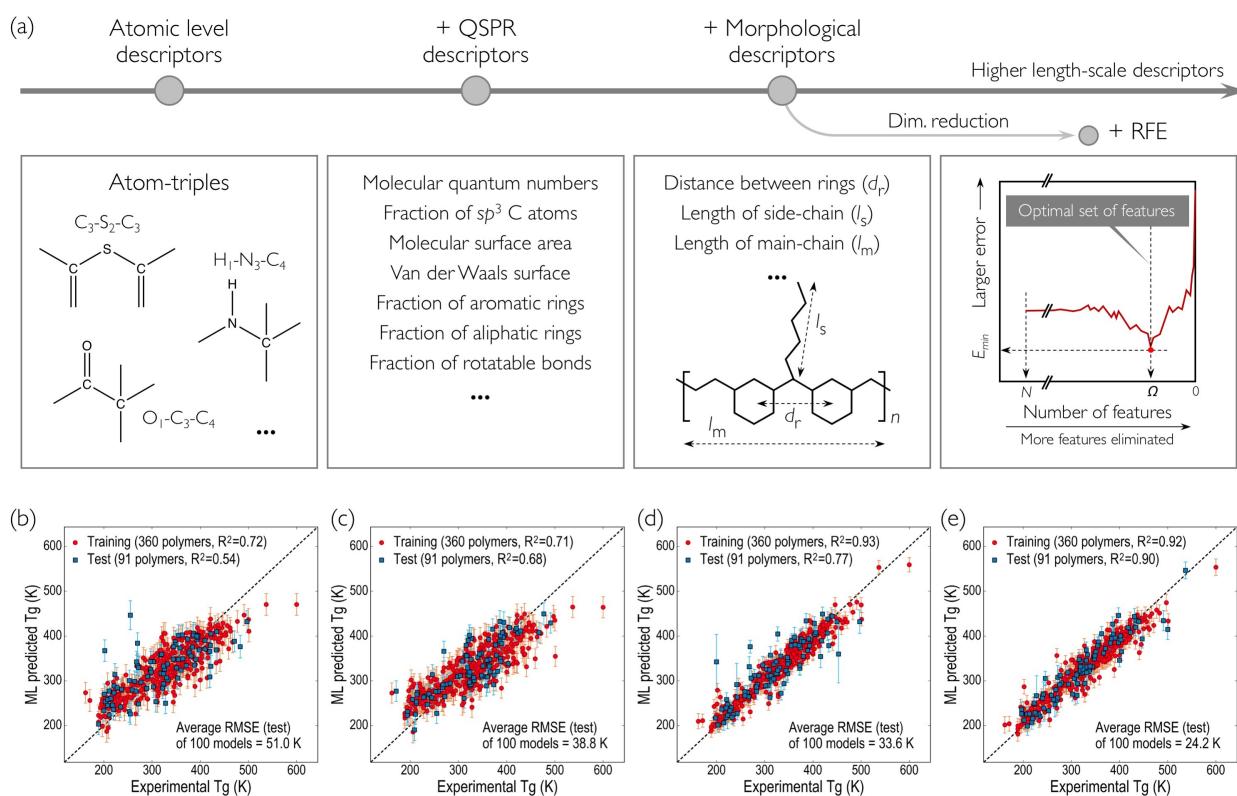


Figure 3: Hierarchy of descriptors used to fingerprint the polymers, and an example demonstration for the systematic improvement of model performance depending on the type of fingerprint considered. (a) Classification of descriptors according to the physical scale and chemical characteristics are shown with representative examples. Dimension of the fingerprint in each level can be reduced by a recursive feature elimination (RFE) process. In the '+RFE' panel, N , Ω , and E_{min} are total number of features in fingerprint, optimal number of features determined by RFE, and minimum error of prediction model, respectively. Plots at the bottom panel show the performance of machine learning prediction models for glass transition temperature (T_g) with (b) only atomic level descriptors, (c) atomic level and QSPR descriptors, and (d) entire fingerprint components including morphological descriptors. (e) shows how the optimal subset selected by RFE improves the prediction model for T_g .

morphological descriptors. The overall fingerprint of a polymer is constructed by concatenating the three classes of fingerprint components. In total, this leads to a fingerprint with 229 components. Subsequently, we show that the dimensionality of the fingerprints needs to be reduced to improve prediction performance. Also, during performance assessment, we use different combinations of fingerprint components. For clarity of that discussion, we introduce some nomenclature. The atom triples fingerprint, QSPR descriptors, and morphological descriptors are, respectively, denoted by ‘A’, ‘Q’, and ‘M’. Therefore, ‘AQ’ implies a combination of just the atom-triples and QSPR descriptors.

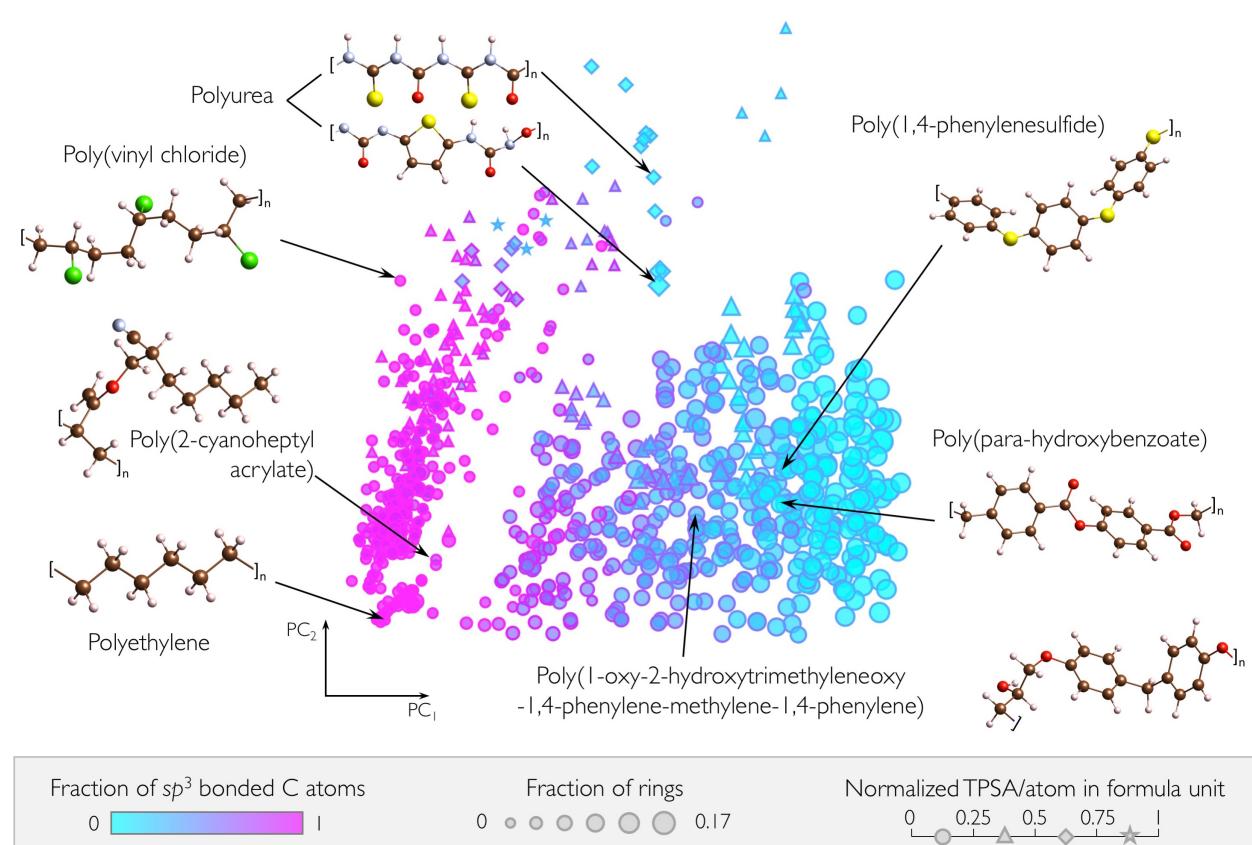


Figure 4: Graphical summary of chemical space of polymers considered. 854 chemically unique organic polymers generated by structure prediction method (minima-hopping⁵⁹) and experimental sources^{36,37} distributed in 2D principal component space. Two leading components, PC_1 and PC_2 , are produced by principal component analysis, and assigned to axes of the plot. Fraction of sp^3 bonded C atoms, fraction of rings, and normalized TPSA per atoms in a formula unit are used for color code, size and symbol of each polymer. A few representative structures with various number of aromatic and/or aliphatic rings and their position on the map are shown.

In order to visualize the chemical diversity of polymers considered here, we have performed principal component analysis (PCA) of the complete fingerprint vector. PCA identifies orthogonal linear combinations of the original fingerprint components that provide the highest variance; the first few principal components account for much of the variability in the data.⁷ Figure 4 displays the dataset with the horizontal and vertical axes chosen as the first two principal components, PC₁ and PC₂. Molecular models of some common polymers are shown explicitly, and symbol color, symbol size and symbol type are used to represent the fraction of *sp*³ bonded C atoms, fraction of rings, and TPSA of polymers, respectively. As an example from the figure, PE is composed of only *sp*³ bonded C without any rings in the chain, while poly(1,4-phenylene sulfide) contains no *sp*³ bonded C atoms, and more than 90% of its atoms are part of rings. As a result, these two polymers are situated far from each other in 2D principal component space.

4 Surrogate (machine learning) model development

4.1 Recursive feature elimination

As alluded to earlier, our general fingerprint is rather high in dimensionality, and not all of the components may be relevant for describing a particular property. In fact, irrelevant features often lead to a poor prediction capability. On the practical side, large fingerprint dimensionality also implies longer training times. There is thus a need to determine the optimal subset of the complete fingerprint necessary for the prediction of a particular property (i.e., different properties may require different subsets of the fingerprint vector). Rather than manually deciding which fingerprint components to use, one may utilize a wide variety of dimensionality reduction techniques to automatically select a set of features that best represent a particular property. In the current work, we utilize the recursive feature elimination (RFE) algorithm to sequentially eliminate the least important features for a given property.⁶⁰ The RFE is an iterative procedure for reducing the number of features by re-

cursively repeating the estimation of feature ranking (importance) and elimination of the least important feature. The rightmost panel of Figure 3a demonstrates how the optimal set of features were determined as the best fingerprint components by RFE. A simple linear model was used to rapidly remove unwanted features and the final set of features is passed forward to the non-linear machine learning algorithm described next in Sec 4.2. The final set of features selected by RFE can also be used to obtain an intuitive understanding of how certain key fingerprint components influence particular materials properties.

4.2 Gaussian process regression

In our past work,^{6,13,26} we have successfully utilized kernel ridge regression (KRR)⁶¹ to learn the non-linear relationship between a polymer's fingerprint and its properties. However, in this work we utilize GPR because of two key benefits. Firstly, GPR learns a generative, probabilistic model of the target property and thus provides meaningful uncertainties/confidence intervals for the prediction. Secondly, the optimization of the model hyperparameters is relatively faster in GPR because one may perform gradient-ascent on the marginal likelihood function as opposed to the cross-validated grid-search which is required for KRR. We use a radial basis function (RBF) kernel defined as

$$k(\mathbf{x}_i, \mathbf{x}_j) = \sigma^2 \exp \left[\frac{-(\mathbf{x}_i - \mathbf{x}_j)^2}{2l^2} \right] + \sigma_n^2 \delta(\mathbf{x}_i, \mathbf{x}_j), \quad (1)$$

where σ , l , and σ_n are hyperparameters to be determined during the training process (in the machine learning parlance, these hyperparameters are referred to as signal variance, length scale parameter and noise level parameter, respectively). \mathbf{x}_i and \mathbf{x}_j are the fingerprint vectors for two polymers i and j . (\mathbf{x}_i is an m dimensional vector with components $x_i^1, x_i^2, x_i^3, \dots, x_i^m$, determined and optimized by the RFE step described above). Performance of the model was evaluated based on the root mean square error (RMSE) and the coefficient of determination (R^2). During the surrogate model development step using GPR, including substeps for

selection of the best combination of fingerprint types, and optimization of dimensionality of the fingerprint by recursive feature elimination (RFE), 80% of the data was used for training and the remaining 20% was set aside as a test set. Learning curves for machine learning models for each property are shown in Figure S1.

4.3 Optimization of fingerprint vector

Certain properties, like the DFT computed atomization energy, depend mainly on the connectivity of the atomic species and only weakly on the morphology. As a result, we were able to achieve a test-RMSE of 0.01 eV using just ‘AQ’ components. However, properties such as T_g are dependent not only on the atomic-species and bonding but they are also strongly influenced by the morphology of the polymer. In Figure 3b, we see how using just the atom-triplet fingerprint components results in a poor model for the T_g with a significantly high RMSE of 51 K. However, adding the QSPR descriptors results in a visible improvement of the model performance, resulting in an RMSE of 39 K.(Figure 3c) Two examples of QSPR descriptors which are highly correlated with T_g are the fraction of rotatable bonds (Pearson correlation -0.66) and the fraction of ring atoms (Pearson correlation +0.63). As the fraction of rotatable bonds is increased, the polymer chains become more flexible, thus resulting in a decrease in T_g . The fraction of rings is positively correlated with T_g due to fact that rings increase the stiffness of the polymer chain thus reducing inter-chain mobility. The addition of the morphological fingerprints like the number of side-chains and the shortest topological distance between rings further improves the predictive capability of the model.(Figure 3e) However, after including all hierarchical levels of the fingerprint, the dimensionality of the fingerprint vector becomes unnecessarily large (229). Subjecting these combined set of fingerprints to RFE brings down the dimensionality to 69. Through this systematic process of fingerprint development the final test-RMSE for T_g is brought down to 24.2 K.(Figure 3e)

Similarly, other experimental properties like the solubility parameter and density showed a strong dependence on the ‘Q’ or ‘M’ type fingerprints. For some cases, the feature elimina-

tion process reduces the number of fingerprints to no more than a dozen or so. For instance, in the case of the refractive index, 19 fingerprint components are sufficient to obtain a good model.

5 Model performance validation

The final machine learning models for each of the properties under consideration here were constructed using the entire polymer dataset for each property. To avoid overfitting the data, and to ensure that the models are generalizable, we employed 5-fold cross-validation, wherein the dataset is divided into 5 different subsets and one subset was used for testing while remaining sets were employed for training. Table 1 summarizes the best fingerprint, dimension of fingerprint vector, and performance based on RMSE for the entire dataset.

Table 1: Summary of fingerprint used for development of machine learning prediction model, and the performance of prediction for each property. Best fingerprint is selected based on average RMSE of test-set for 100 models. (A: Atomic level descriptors, Q: QSPR descriptors, M: Morphological descriptors, +RFE: subject to the RFE process)

Property	Best fingerprint	Dimension of fingerprint	RMSE
Bandgap	AQM + RFE	88	0.30 eV
Dielectric constant	AQ + RFE	35	0.48
Refractive index	AQM + RFE	19	0.08
Atomization energy	AQ	207	0.01 eV/atom
Glass transition temperature	AQM + RFE	69	18 K
Solubility parameter	AQM + RFE	24	0.56 MPa ^{1/2}
Density	AQ + RFE	9	0.05 g/cm ³

Parity plots in Figure 5 are shown to compare experimental or DFT computed properties with respect to machine learning predicted values with percentage relative error distribution. Several error metrics, such as RMSE, mean absolute error (MAE), mean absolute relative error (MARE) and $1-R^2$ were considered to evaluate the performance of these models, and

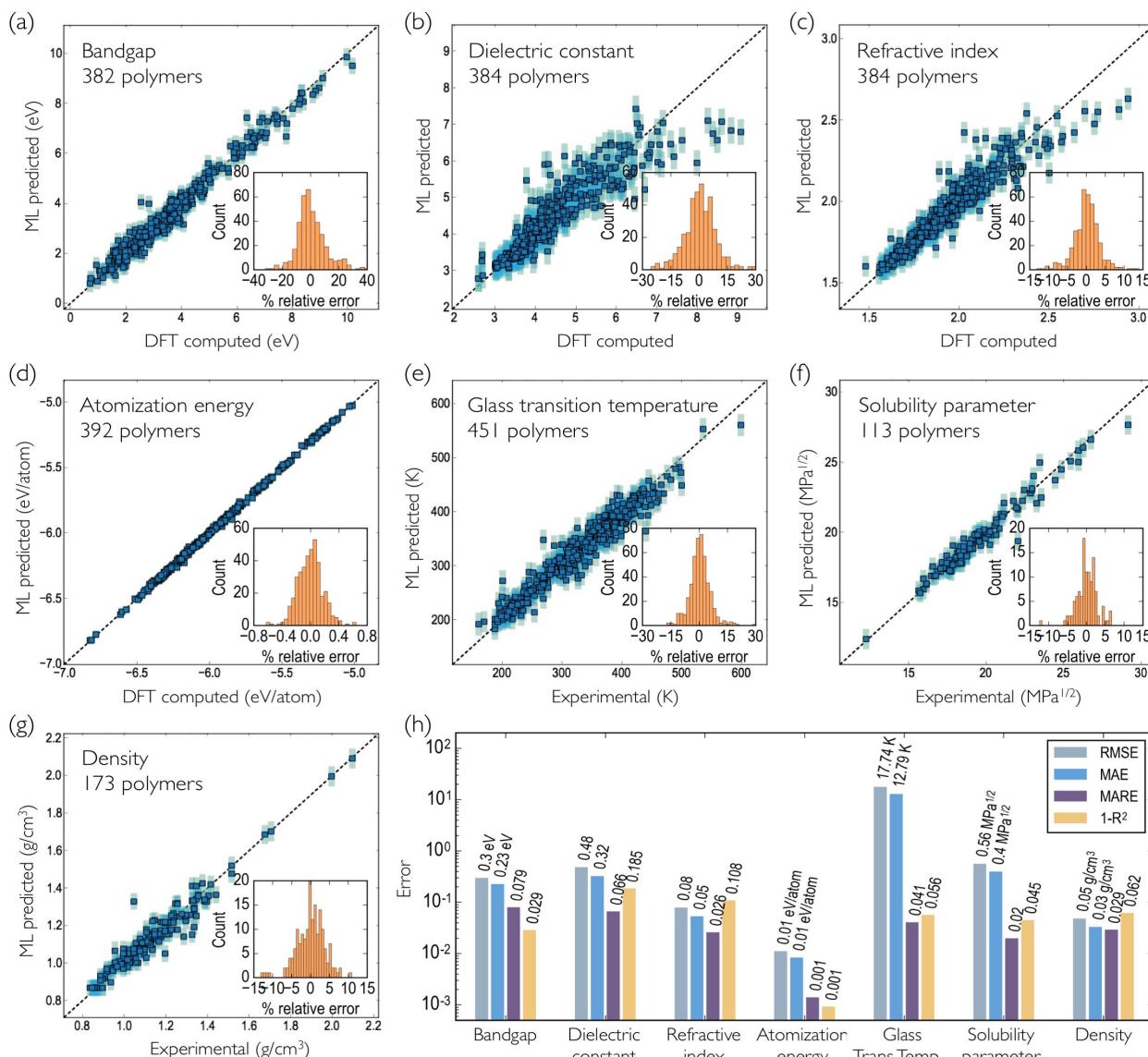


Figure 5: The performance of the cross-validated machine learning models developed by GPR with combination of RBF and white noise kernels. Comparison of DFT computed (a) bandgap, (b) dielectric constant, (c) refractive index, (d) atomization energy, experimental (e) T_g , (f) Hildebrand solubility parameter, and (g) density for the predicted values are shown with inset of distribution of % relative error, $(y - Y)/Y \times 100$ where Y is DFT computed or experimental value, and y is machine learning predicted value. Other error metrics including RMSE, mean absolute error (MAE) and mean absolute relative error (MARE) and $1 - R^2$ are summarized in (h).

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8 6 Polymer Genome online platform 9

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11 For easy access and use of the prediction models developed here, an online platform called
12 Polymer Genome has been created. This platform is available at www.polymergenome.org.⁶²
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14 The Polymer Genome application was developed using Python and standard web languages
15 such as Hypertext Preprocessor (php) and Hypertext Markup Language (HTML). As user
16 input, the repeat unit of a polymer or its SMILES string may be used (following a prescribed
17 format described in the Appendix). One may also use an integrated drawing tool to sketch
18 the repeat unit of the polymer.
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21 Once the user input is delivered to Polymer Genome by the user, property predictions
22 (with uncertainty) are made, and the results are shown in an organized table. The names of
23 polymers (if there are more than one meeting the search criteria) with SMILES and repeat
24 unit are provided with customizable collection of properties. Upon selection of any polymer
25 from this list, comprehensive information is reported. This one-page report provides the
26 name and class of the polymer, 3D visualization of the structure with atomic coordinates (if
27 such is available), and properties determined using our machine learning models. A typical
28 user output of Polymer Genome is captured in Figure 6.
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43 7 Challenges and opportunities 44

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46 Polymer Genome, including the dataset, fingerprinting scheme, and machine learning models,
47 remain in early stages. Coverage of the polymer chemical space needs to be progressively
48 increased, and further developments in the fingerprinting scheme is necessary to adequately
49 capture conformational (e.g., *cis* versus *trans*, tacticity, etc.) and morphological features
50 (e.g., copolymerization, crystallinity, etc.). Any topological or morphological variations that
51 cannot be well represented by purely the repeat unit of the polymer (such as irregular
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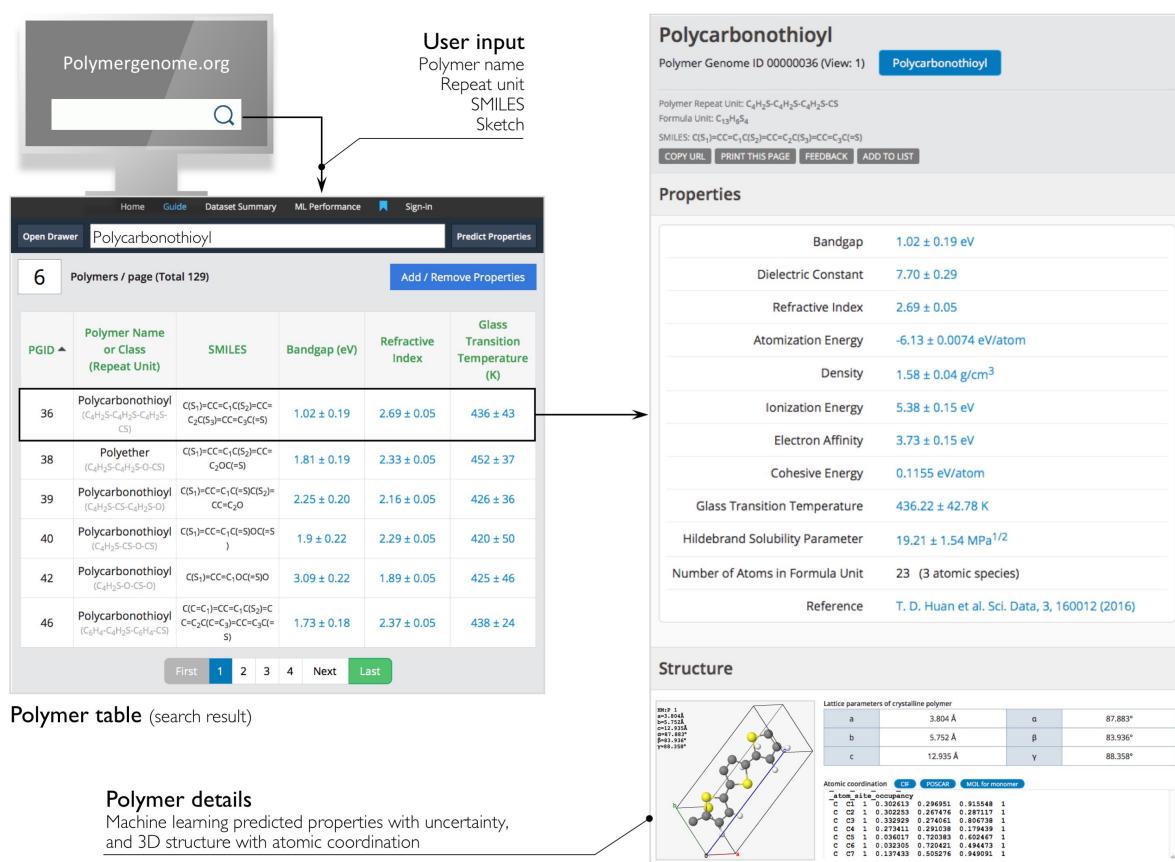


Figure 6: Overview of Polymer Genome online platform available at www.polymergenome.org. Keyword Polycarbonothiolyl is used as an example user input to show resulting Polymer table, and Polymer details page of selected polymer among the list.

side-chains in low-density polyethylene, or cross-linking) would indeed require macro-level descriptors to capture variations in the property space. One such macro-level descriptor could be the experimentally measured density itself.

While our implementation currently reports the Bayesian uncertainty of a particular property prediction, it would also be crucial to carefully investigate the uncertainties and errors associated with the underlying experimental measurements. In many cases, properties such as the T_g are reported as a range rather than a single absolute value and in some cases there is a significant variation in the measured property depending on the specific experimental technique utilized. A detailed analysis is currently underway to develop a framework to quantify these intrinsic uncertainties.

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3 Going forward, the process of inverse design, or the autonomous suggestion of materials
4 candidates with user-requested properties, would be an invaluable addition to any materials
5 informatics platforms and preliminary progress on this front has been reported in an earlier
6 work.¹³ Systematic pathways to achieve such expansions are presently being examined to
7 extend the applicability of the polymer informatics paradigm to a wide range of technological
8 domains.
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17 8 Conclusions

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21 The Materials Genome Initiative and similar other initiatives around the world have provided
22 the impetus for data-centric informatics approaches in several subfields of materials research.
23 Such informatics approaches seek to provide tools and pathways for accelerated property pre-
24 diction (and materials design) via surrogate models built on reliable past data. Here, we
25 have presented a polymer informatics platform capable of predicting a variety of important
26 polymer properties on-demand. This platform utilizes surrogate (or machine learning) mod-
27 els that link key features of polymers (i.e., their “fingerprint”) to properties. The models are
28 trained on high-throughput DFT calculations (of the bandgap, dielectric constant, refractive
29 index and atomization energy) and experimental data from polymer data handbooks (on
30 the glass transition temperature, solubility parameter and density). Certain properties, like
31 the atomization energy, depend mainly on the atomic constituents and short-range bonding,
32 whereas other properties, such as the glass transition temperature, are strongly influenced
33 by morphological characteristics like the chain-stiffness and branching. Our polymer fin-
34 gerprinting scheme is thus necessarily hierarchical and captures features at multiple length
35 scales ranging from atomic connectivity to the size and density of side chains. The prop-
36 erty prediction models are incorporated in a user friendly online platform named Polymer
37 Genome (www.polymergenome.org), which utilizes a custom Python-based machine learning
38 and polymer querying framework.
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Appendix: User input interface

The Polymer Genome online platform accepts multiple types of user inputs. These user inputs are converted to fingerprints which are in turn used by the surrogate models to obtain property predictions. The first type of user input is the name of the polymer. We have attempted to preserve compatibility with many different naming conventions such as the formula unit, common name, structure based name, and other commonly accepted abbreviations for each polymer. For instance, polyethylene, can be queried by submitting any one of the following names: PE, C₂H₄ and polyethylene. It is also convenient to represent polymers through a string of concatenated building blocks which make up its repeat-unit. For example, PE and polyethylene terephthalate (PETE) can be written as CH₂-CH₂ and C₆H₄-CO-O-CH₂-CH₂-O-CO, respectively. Here we use the symbol ‘-’ to imply the connection of neighboring blocks. The current version of the Polymer Genome application can handle the following building blocks: CH₂, CH, O, CS, CO, NH, C₆H₄, C₄H₂S, C₅H₃N, C₄H₃N, CF₂, CF, CHF, CC₁₂, CC₁, CHCl, CBr₂, CBr, CHBr, Cl₂, CI and CHI. (Figure S2)

Table 2: Example polymers specified by multiple input types.

Input type	Example			
Polymer name	Polyethylene, PE, C ₂ H ₄	Polyethylene terephthalate, PETE, C ₁₀ H ₈ O ₄		Polythiophene, C ₄ H ₂ S
Repeat unit	CH ₂ , CH ₂ -CH ₂ , ...	CH ₂ -CH ₂ -O-CO-C ₆ H ₄ -CO-O		C ₄ H ₂ S, C ₄ H ₂ S-C ₄ H ₂ S, ...
SMILES	CC	CCOC(=O) C(C=C ₁)=CC=C ₁ C(=O)O	C(S ₁)=CC=C ₁	[*]C(S ₁)=CC([*])=C ₁
Sketch				

There are several other schemes, proposed in earlier studies, to represent the structure of polymers, such as Wiswesser line-formula notation (WLFN),^{63,64} SMARTS,⁶⁵ MDL Molfiles,⁶⁶ etc. Among these representations, Polymer Genome is capable of handling the SMILES format, a powerful representation to describe the topological structure of molecular

systems.⁶⁷ Since SMILES was originally developed for isolated molecules, we have introduced the following custom variations to extend its applicability to polymers: 1) If not specified, the first and last atoms in the main-chain of the SMILES are the linking atoms of the polymer chain. 2) Atoms other than the first and last can also be assigned as the linking atoms by adding the special symbol, [*], next to the atom symbol. For example, C(S1)=CC=C1 is obviously the SMILES of polythiophene with interconnection between the first and the last C atoms, while [*]C(S1)=CC([*])=C1 has different connectivity between neighboring rings. This difference of connectivity for these two variants of polythiophene can be seen in Table 2. Here, symbol '=' is used to indicate a double bond between adjacent atoms. Following conventional SMILES notation, triple bonds are specified by '#'. Branches/side-chains are specified using brackets (). Numbers beside the atom symbols indicate that the atoms associated with the same number are connected to each other. S1 and C1 from above examples are connected ring-atoms thus showing how the thiophene ring can be illustrated through the linear connection of atom symbols in SMILES.

The most convenient way for users to search/query any polymer is to draw the repeat-unit using the sketcher tool (structure editor) provided by Polymer Genome. This 2D topological sketch can be converted on-the-fly to the SMILES format with help of JSME Molecule Editor toolkit⁶⁸ as implemented in the search-interface of Polymer Genome. Four types of acceptable user input are summarized with examples of PE, PETE, and two different structures of polythiophene in Table 2. The sketching utility and SMILES are especially useful for crafting polymers with complex connectivity or for those cases in which the predefined repeat-units are not sufficient to represent the desired polymers. Having the flexibility to choose from multiple user input formats, makes the Polymer Genome online platform a versatile digital assistant for polymer applications.

Supporting Information Available

Figure S1. Learning curves constructed from the RMSE of the machine learning models.
For each model, data was obtained from 100 independent runs.

Figure S2. Building blocks implemented in Polymer Genome for constructing polymer repeat units.

This material is available free of charge via the Internet at <http://pubs.acs.org/>.

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Corresponding Author

E-mail: rampi.ramprasad@mse.gatech.edu (R. Ramprasad).

Notes

C. Kim and A. Chandrasekaran contributed equally to this work. All authors participated in the writing of the manuscript.

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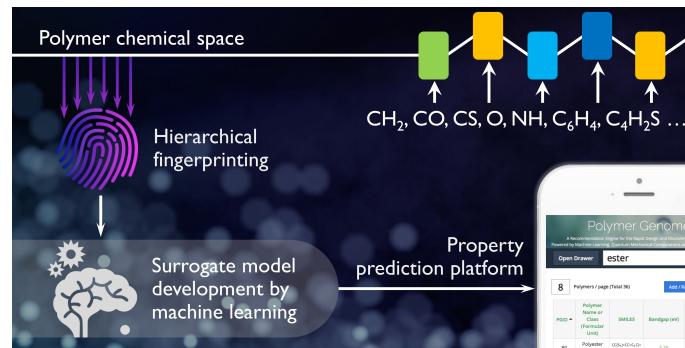
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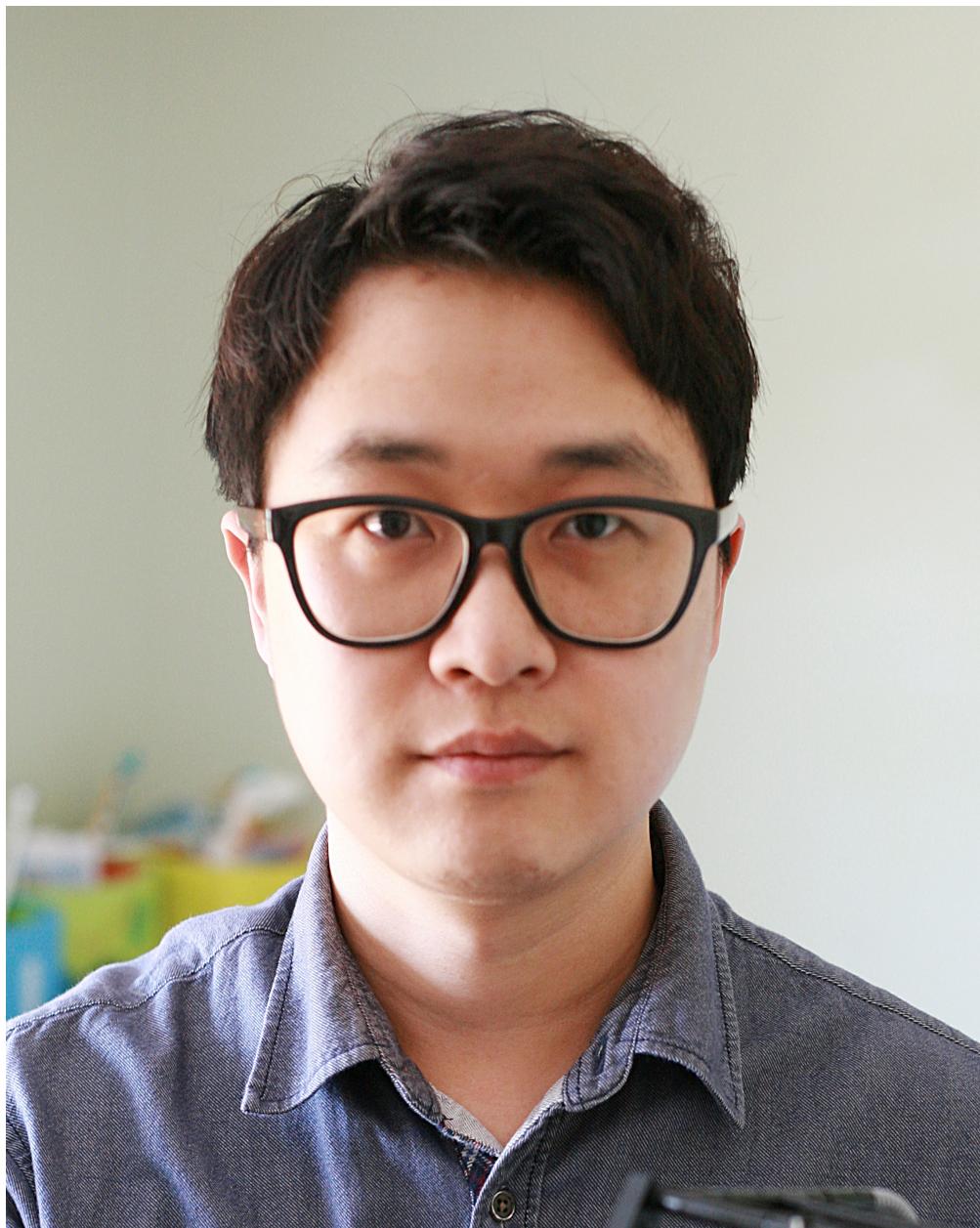
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Graphical TOC Entry



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3 **Chiho Kim** is a research engineer in School of Materials Science and Engineering, Georgia
4 Institute of Technology. He obtained a Ph.D. from Hanyang University, South Korea in 2009,
5 and worked for Samsung Electronics until 2014. From 2014 to 2018, he was a postdoctoral
6 fellow and research associate at the University of Connecticut. His current research interests are
7 in applying machine learning techniques to a variety of material classes to accelerate the design
8 and discovery of advanced materials.
9



Anand Chandrasekaran is a postdoctoral fellow in the School of Materials Science and Engineering, Georgia Institute of Technology. He received his Ph.D. from EPFL, Switzerland in 2016 for his thesis on the ab initio and experimental study of defects and domain walls in ferroelectric oxides. From 2016 - 2018 he was a postdoc at the University of Connecticut. His current interests include applying state-of-the-art machine learning techniques to a wide range of materials science challenges.



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2
3 **Tran Doan Huan** received his PhD in Physics from Florida State University in 2010. He is now
4 postdoc fellow at the University of Connecticut after completing a postdoc at the University of
5 Basel (Switzerland) where he started his current interest in advanced computational approaches
6 (electronic structure and machine learning) in materials science.
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Deya Das is a postdoctoral fellow in School of Materials Science and Engineering, Georgia Institute of Technology. She received her Ph.D. degree from Materials Research center, Indian Institute of Science, India for her thesis on Li storage studies in graphitic materials through tuning of electronic structures. Her current work is focused towards understanding of Li diffusion in polymer electrolyte for Li ion batteries.



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2
3 **Prof. Rampi Ramprasad** is presently the Michael E. Tennenbaum Family Chair and the
4 Georgia Research Alliance Eminent Scholar in Energy Sustainability in the School of Materials
5 Science and Engineering at Georgia Institute of Technology. Prior to joining Georgia Tech, he
6 held positions at the University of Connecticut and Motorola's R&D laboratories at Tempe, AZ.
7 Prof. Ramprasad received his B. Tech. in Metallurgical Engineering at the Indian Institute of
8 Technology, Madras, India, an M.S. degree in Materials Science & Engineering at the
9 Washington State University, and a Ph.D. degree also in Materials Science & Engineering at the
10 University of Illinois, Urbana-Champaign. Prof. Ramprasad's area of expertise is in the
11 development and application of atomistic and data-driven materials computational tools, and
12 more broadly in the utilization of such methods for the design and discovery of new materials,
13 especially dielectrics and catalysts. Prof. Ramprasad is a Fellow of the American Physical
14 Society, an elected member of the Connecticut Academy of Science and Engineering, and the
15 recipient of the Alexander von Humboldt Fellowship and the Max Planck Society Fellowship for
16 Distinguished Scientists.



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