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Predictive Approaches for 3D-Printing: Methods and Approaches for Polymeric Materials

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ABSTRACT

By bridging molecular-level insights with macroscopic performance metrics, computational strategies are poised to transform how we design next-generation 3D-printable materials with enhanced precision, functionality, and sustainability. We present a critical overview examining the role of computational methods in advancing the design and application of 3D-printable polymers. We cover key considerations—including solvation behavior, viscosity, gel point, mechanical properties, and polymer structure—as well as the design of new polymer functionalities. We highlight how a spectrum of physics-based methods, ranging from quantum chemical to coarse-grained simulations, can be leveraged to interrogate relevant polymer properties at multiple scales. In particular, we illustrate the growing impact of machine learning in accelerating polymer discovery and optimization. Such methods, whether applied independently or integrated into multi-scale modeling frameworks, offer powerful tools for prescreening and selecting optimal formulations tailored to diverse 3D printing technologies and applications. Although challenges remain to integrate different approaches into workable prediction pipelines, the rate of advance and improvements in methods, data interoperability, and data quality, offer great promise of a 'concept to print' pipeline in the future.

This article is categorized under:

Structure and Mechanism > Computational Materials Science

Data Science > Artificial Intelligence/Machine Learning

Structure and Mechanism > Molecular Structures

1 | Introduction

Additive manufacturing (AM), commonly referred to as 3D printing, is gaining increasing traction in polymer processing. There have been significant advances in producing customized components for biomedical devices [1, 2], chemical reactors [3–6], lightweight structural parts in aerospace [7, 8], and rapid prototyping in various industries [9–11]. Further development in this area can be aided by efficient organization of relevant polymeric and formulation property data, hand-in-hand with predictive modeling, to allow guided selection, design, and tuning of reactants, chemical properties

and manufacturing processes. As the field grows, it is therefore necessary to take stock of state-of-the-art modeling and data engineering methods, critically assessing their past and potential future uses as applied to polymers and 3D printing. While there have been a number of polymer studies predicting properties relevant to 3D printing, organizing these studies in context and increasing direct focus on 3D printing and its specific applications will be important future directions of the field.

Polymers represent a class of materials of significant scientific and industrial importance in their own right due to their diverse and adaptable properties [12–18]. Polymer processing by 3D printing involves techniques which can be broadly split into light-based and extrusion-based options. Light-based techniques, including stereolithography (SLA), selective laser sintering (SLS), and volumetric additive manufacturing (VAM), selectively induce reactions and manufacture parts typically using UV. Extrusion-based options, such as fused deposition modeling (FDM), involve controlled release of a melted filament from a nozzle to build up fused layers. These methods allow for precise control over the dimensions of printed parts, including at very small length scales, with resolutions often reaching the microscale [19]. Printing control can in principle be enhanced by appropriate modeling techniques, which can aid fine-tuning of printability and mechanical, thermal, and chemical properties of printed parts [20], including elasticity, tensile strength, thermal stability, resistance to environmental degradation, and biocompatibility [21].

Fully leveraging modeling to tune polymer and formulation properties for 3D printing hinges on predictive understanding of the interplay between monomer chemical composition and large-scale behavior. Since polymers are long-chain molecules formed by polymerization between smaller monomer units, comprehensive polymer modeling must cover functionality at several time and length scales, stemming from a variety of chemical phenomena [22], including functional group interactions, branching, and cross-linking [23]. In addition to property modeling, discovery of new polymers presents a particularly complex challenge, largely due to the high dimensionality of the design space [24, 25]. Seeking optimal performance across various service environments adds complexity, making it difficult to make informed design choices beforehand, but successful modeling and computational discovery may ultimately yield atomistic and mechanistic insight that is difficult to obtain using experimental techniques [26–29]. Modeling can be used to pre-screen polymers, monomers, or formulations, directing experimental efforts toward promising options, circumventing the need for extensive experimental trial and error, and reducing the necessity for resource-intensive, labor-intensive, environmentally-intensive, or unsafe procedures [30, 31]. This relies on established knowledge of available methods and their applicability in the complex polymer space.

Available methods include both computational chemistry techniques grounded in physical principles, and data-based statistical methods. Researchers take advantage of various models, representations of molecules, data sources, and data processing techniques. Methods grounded in underlying chemistry and physics range in computational cost and accuracy from first-principles solutions of the Schrödinger equation to empirically fitted coarse-grained force fields. Further abstraction is seen with heuristic models. These extend to machine learning (ML) and artificial intelligence (AI), which have emerged as powerful predictive tools for data-driven multi-physics modeling in polymer discovery, offering a more efficient approach to navigating the intricate design landscape [32, 33]. Integrating experimental data and computer simulations has generated a vast amount of information, paving the way for applying ML algorithms in materials science. Utilizing reasonable amounts of experimental data within an ML framework enables the development of quantitative structure–property relationships (QSPRs) for predicting desired polymer properties [34]. Additionally, the emergence of generative AI enables new versatility in materials design and inverse polymeric engineering [35]. This range of physics-based and data-based models is illustrated in Figure 1. Navigating these tools to select a model or combination of models is a vital part of any polymer modeling task [23, 29], which must be undertaken in the context of the system of interest, properties to be predicted, and available data. For example, study of electronic properties requires quantum chemistry methods, while if a researcher has access to a large volume of relevant experimental information, data-driven techniques may prove more useful.

Here, we examine and showcase current computational chemistry and data-driven modeling techniques for polymers and related systems in the context of their applicability to guiding design and selection of 3D printable formulations and parts. We discuss several recent case studies exemplifying the use of different aspects of modeling in this field, critically assessing the methods available, their advantages and disadvantages, and where and how they can best be applied. To achieve this, we consider several properties which relate to 3D printing processes. For example, solubility and solution interactions are important in polymer processing [22] and printing formulation design [22, 36, 37]. Meanwhile, formulation viscosity impacts effectiveness and efficiency of printing, whether by extrusion or light-based methods [36–38]. Structural and tensile properties of printed parts are also important [39], as is the accuracy of the reproduction of desired dimensions (print fidelity) [40].

We structure the discussion and analysis by method. We first address situations in which different computational chemistry methods have been used, beginning with a discussion of molecular representation, then turning to quantum chemistry methods and then to several types of force field method. We then discuss data-driven polymer discovery methods. We outline the polymeric data sources and preparation steps, followed by a discussion of polymer informatics. We present examples of both traditional machine learning methods and generative AI applied to polymer research. We specifically address the integration of these approaches with 3D printing manufacturing. We then discuss the remaining challenges and future directions following this analysis. We highlight cases in which these methods have been used to make predictions directly relating to AM processes, as well as other cases where they have been applied to printable polymers and properties relevant to AM. Finally, we provide a critical summary of all the method types addressed and their applicability to 3D printing. We thereby illustrate and

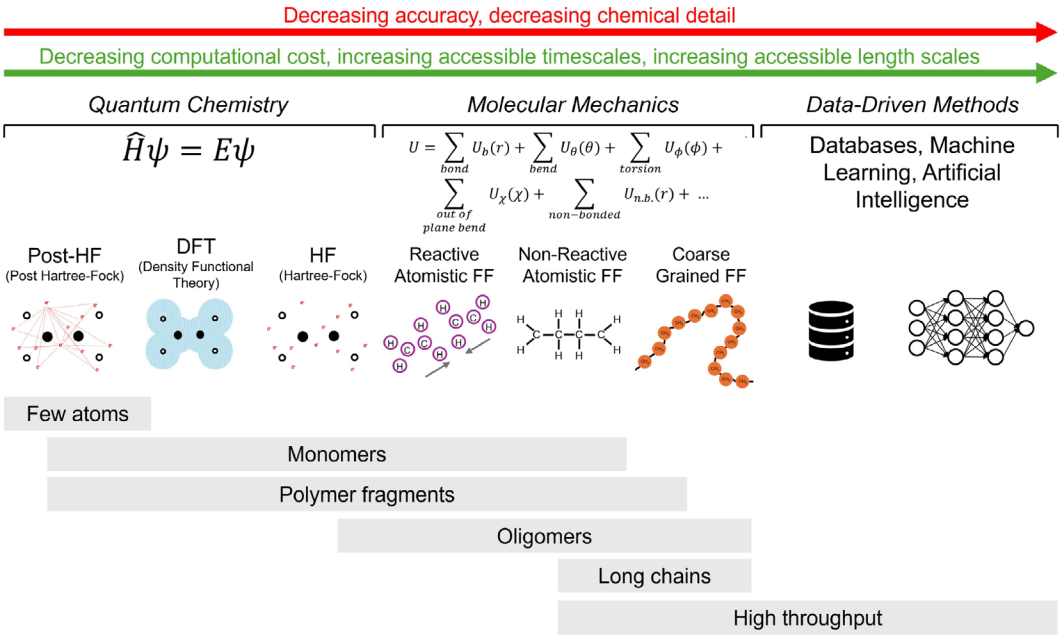

FIGURE 1 | Illustration of different quantum chemistry modeling techniques, their approximate accuracy/cost hierarchies, and the kinds of systems and tasks that each is suited to.

evaluate currently available methods and studies, and comment on future directions for the evolution of the field.

2 | Physics-Based Modeling

Traditionally, polymer modeling involves simulations whose principles are grounded in some combination of fundamental chemistry and empirical observations. This can provide insight into 3D printing processes, predicting and explaining features of printed materials, the polymerization printing processes, and ink formulations. Simulations can be applied to specific systems for granular insight, or in a high-throughput manner, computationally testing several candidate systems to expedite formulation design. Advantages of physics-based models include explainability and chemical detail stemming from their direct link to underlying phenomena. However, methodological compromises are necessary to make large and complex polymer systems computationally tractable. Methods grounded in data (discussed in Section 3) can be applied on a larger scale to materials exploration and discovery.

Like any computational chemistry task, polymer simulation involves a model describing energy and forces, and a simulation method that yields thermodynamic information based on the underlying model. Simulation methods described in textbooks and throughout the literature [41–44] may be used for polymer modeling [45, 46]. Prominently, Molecular Dynamics (MD) examines evolution in time via Newton's equations of motion [41, 42]. In principle, MD could provide a comprehensive picture of a system given enough time. However, statistically rare events are unlikely to be accessed during a standard MD simulation. These include structural and conformational conversions, alongside slow-timescale annealing and reorganization, which can be crucial for understanding polymer properties due to the significant importance of polymer secondary structure [47]. Enhanced sampling algorithms can access rare events [41, 48], including in polymer conformation searching [44, 47].

Simulations rely on the ability of the underlying model to reproduce the physics of particle interactions. Over the past century, a wide range of relevant models have been developed [49–54], with a trade-off between accuracy and detail on the one hand and computational cost on the other, as illustrated in Figure 1. When selecting a model for polymer simulations, minimizing computational cost to cover long simulation times and large, complex systems is of high importance. However, computationally cheap atomistic or coarse-grained [55] force fields are not always sufficient to describe relevant interactions. The polymerization reaction process impacts properties [49], while the electronic structure of electronically conductive polymers dictates function [50], but neither is accounted for using standard force fields. This necessitates the use of costlier reactive force fields [49, 51] or quantum chemistry [52]. Meanwhile, classical force fields typical in polymer studies struggle to reproduce specific properties [56], including some transport properties, which require long simulation times not suited to quantum chemistry. ML can be a powerful tool combined with traditional simulation principles, with force fields trained using ML [57] targeting quantum accuracy at close to force field cost.

In the following section, we discuss and assess a selection of modeling case studies which use the methods laid out above to either directly address 3D printing or otherwise address properties relevant to the process. The section is arranged according to the type of underlying model used.

2.1 | Conformational Sampling

A molecule's properties depend not only on the atoms it contains and their chemical linkages, but on its precise 3D structure,

known as a conformation or conformer. The effect of accessible conformers on behavior typically increases with size and flexibility, as does the challenge of accessing all relevant conformers. Both are particularly profound for polymers; several simulation procedures relevant to polymeric 3D printing require exploration of conformational space. This exploration is particularly important for methods that treat molecules as static entities [58], though it can also apply to dynamic methods like MD. MD naturally explores energetically accessible conformations, but should begin with a reasonable representation of low energy conformers to allow efficient equilibration, and also requires assignment of partial charges, which is influenced by conformation [59]. As such, an accurate ensemble of molecule conformations is crucial to providing correct simulation parameters and property descriptions.

There are several methods to obtain a conformer ensemble. Popular cheminformatics packages including RDKit [60] and OpenBabel [61, 62] provide conformer generation functionality. RDKit conformer generation is based on the distance geometry method [63], in which interatomic distances are stochastically adjusted within specified bonding rules to create a set of candidate conformers [58, 63, 64]. OpenBabel includes a module, CONFAB [65], which systematically alters torsional angles to cycle through possible conformers, as well as a genetic algorithm conformer generator [62]. These methods rapidly generate ensembles in the context of force field energy calculations. Other fast conformer generation methods similarly utilize force fields alongside geometry-based conformer enumeration [65–67] or generative ML [68].

Initial conformer sets generated by force fields alone are not always sufficiently accurate or general. Several pipelines involve ensemble refinement using quantum chemistry energy calculations to yield diverse ensembles close in energy to the lowest minimum, as illustrated in Figure 2. COSMOtherm [70], a popular tool for implementing the COSMO-RS method (see Section 2.2.3) combines force field generation of an initial ensemble with quantum chemistry refinement; an open-source alternative, openCOSMO-RS [69, 71], uses a similar approach. Moreover, it is not guaranteed that fast cheminformatics methods capture all relevant conformers. Pracht, Bohle, and Grimme [44] developed a Conformer-Rotamer Ensemble Sampling Tool (CREST), which uses semiempirical quantum chemistry energy calculations and metadynamics sampling to exhaustively generate full conformer ensembles. While valuable, this comes at an increased computational cost, and the CREST ensemble has not always been found to reproduce experimental structures more accurately than other ensembles [72].

Much use and assessment of conformer methods [64, 73] has been in the context of small molecules. Ebejer, Morris and Deane [64] compared a selection of conformer methods (RDKit [60], BALLOON [68], CONFAB [65], FROG2 [67] and MOE [74]) examining speed, accuracy, and conformer diversity. They found the optimum approach to depend on circumstances, with the RDKit and CONFAB methods proving strong for reproducing experimental structures, but FROG2 the fastest. Application of conformer methods in the context of small molecules can inform 3D printing studies focusing on formulation properties and design through modeling monomers or other formulation components. For example, Zhang et al. [36] recently studied a number of dithioalkylidenes for incorporation into cross-linked hydrogels. They generated conformer ensembles of different types of dithioalkylidenes using CREST and then used quantum chemistry energy minimization to examine their reactivity for printing in the context of accessible conformer space.

When considering polymeric and printed systems, further considerations are necessary. A wider range of conformational properties covering longer length scales exists for polymers than for small molecules; the globular as well as the chain state is relevant [75]. Polymer conformations influence inter- and intra-chain interactions and chain entanglement, which in turn engender important macroscopic properties [75]. For example, Chen et al. [76] recently observed significant effects of conformations and entanglement of hyaluronic acid on rheological properties of printed gels.

Sampling polymer conformations is not straightforward, and it is computationally too expensive to enumerate full polymer conformer ensembles. Smaller representative structures may be required, and MD trajectories, rather than combinatorial methods, are used to obtain realistic geometries. In the context of polymer solubility prediction, Zhou et al. [28], used diversity criteria to select conformers from MD trajectories of a selection of solvated 2–6 monomer oligomers. In a related study, Silva et al. [77] obtained polymer conformers by the same selection method from MD trajectories of bulk and infinite dilution poly(ethylene glycol). They simulated polymers with molecular weights of up to 1000 g mol^{-1}. Generating conformers of such large species by MD suffers from the disadvantage of being a costly process, with the MD simulations in that work using trajectories of 100 ns.

Faster ways to generate conformers of polymers are desirable, particularly considering the fact that conformer generation tends to be only one step of many in a larger workflow. Recently, conformer generation ML methods have been developed with polymer applicability. Conformer-RL, developed by Jiang et al. [78], is based on the idea that reinforcement learning can perform sampling more efficiently than MD-based alternatives. It can generate conformers for long-chain polymers based on training on successively lengthening oligomer chains. As an example, the method was used to successfully generate conformers for an eight-monomer lignin chain based on training on the exponentially smaller conformational space of chains of up to six monomers [78].

2.2 | Quantum Chemistry Simulations

Quantum mechanics methods account for electronic structure and enable access to underlying reactivity [50, 52]. They are thus relevant to determining rates and mechanisms of monomer reaction during 3D printing, including selectivity of both radical formation and reactions governing the structure of the final polymer, with concomitant impact on material properties. Quantum chemistry is similarly relevant to understanding properties of electronically active 3D printed materials. However, use of quantum methods in polymer chemistry is tempered by high computational cost, limiting the size of molecules to be studied, and necessitating smaller models to represent large systems [52]. A limitation is that these smaller systems may not always accurately reproduce polymer characteristics [52]. This necessitates appropriate benchmarking when these methods are used, and

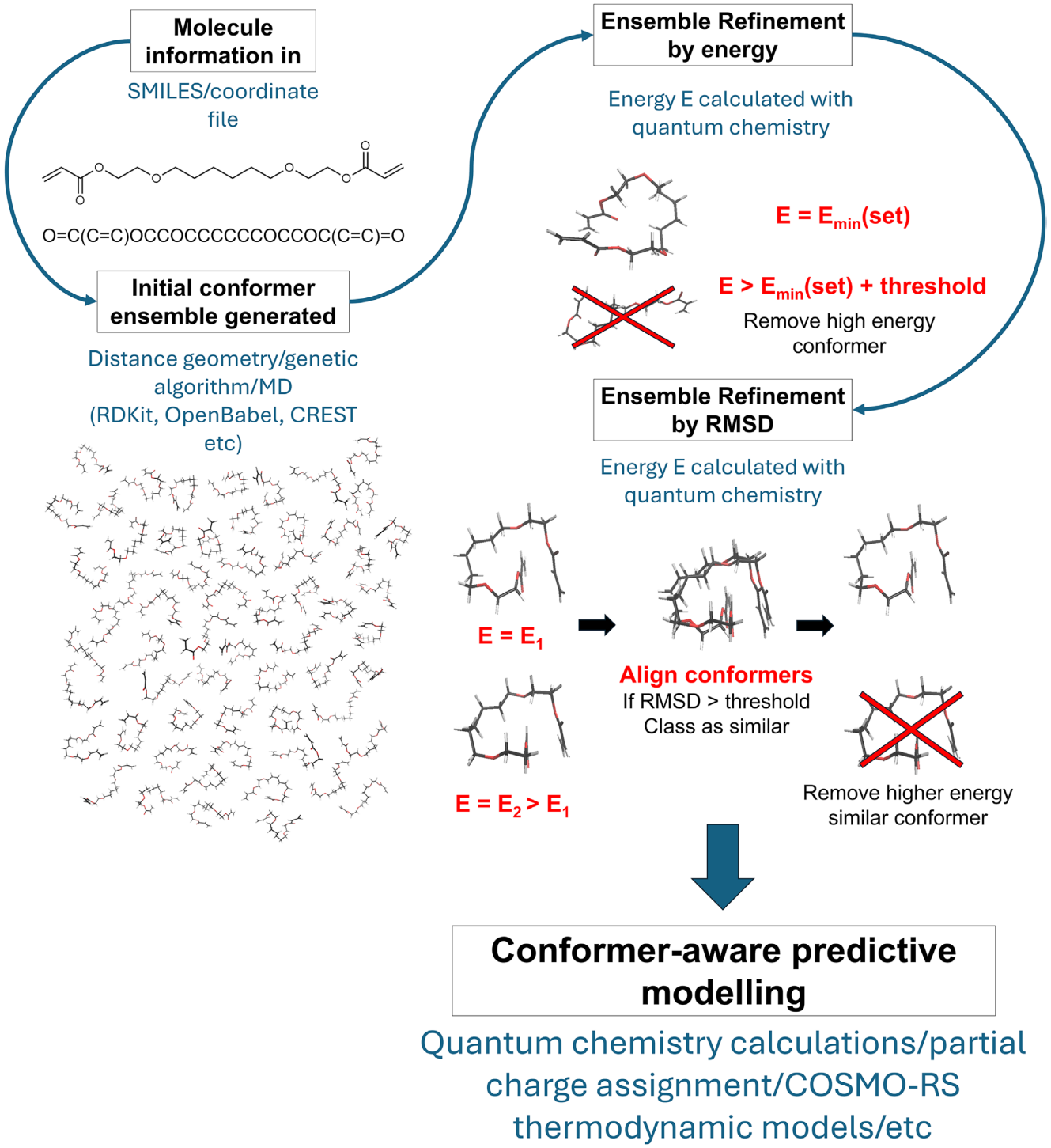

FIGURE 2 | Illustrated conformer pipeline for a sample monomer, hexanediol ethoxylate diacrylate. Initial conformers are generated using geometrical rules, a genetic algorithm, or MD sampling. The ensemble is refined using quantum chemistry to remove high-energy and duplicate geometries. This example applied the openCOSMO-RS conformer pipeline [69], using RDKit [60] for ensemble generation.

has also led to recent development of approaches to mitigate the sources of error [79].

2.2.1 | Reactivity Modeling

In the context of layer-by-layer 3D printing, the rate of polymer formation can be crucial to ensure sufficient adhesion between layers and that the time taken to produce an object is not excessive [80, 81]. For light-driven layerless volumetric printing (VAM) [82], reaction rate versus diffusion plays an important role in driving accurate object formation [83]. The various steps of free radical polymerization (initiation, propagation, chain transfer, and termination) are relevant and must be optimized [52].

Initiation requires an initiator molecule that is photoactive at the desired wavelength. Modeling the light absorption behavior

of an initiator requires electron-aware quantum chemistry approaches. These have a valuable part to play in designing and selecting initiators well-suited to particular absorption wavelengths and formulation systems, but are not yet widely used in this context [84]. Recently, Sun et al. [84] used density functional theory (DFT), a popular choice of quantum chemical method in terms of the trade-off between accuracy and cost, to predict light absorption behavior of a large selection of ketones. They used these predictions to select 10 molecules as promising initiators for wavelengths used in modern printers, and experimentally demonstrated promising behavior of the selected initiators.

Turning to propagation, relative rates of primary reactions to unplanned secondary reactions can inform proliferation of defects within polymerized structures, which impact physical properties of printed parts. Traditional quantum rate constant calculations are well-established; several works in the past decades [52, 85–88] have used them to explore free radical polymerization, including challenging secondary reactions and relative reaction rates, thereby elucidating reaction mechanisms. This includes application to printable systems. For example, Liu et al. [88] studied polymerization of acrylates, common in light-based printing [89], while works of Van Cauter, Van Speybroeck and Waroquier [86], Van Cauter et al. [85] and Cuccato et al. [87] studied polymerization of poly(vinyl chloride), a filament displaying attractive durability, chemical resistance, ductility and strength, but amenable only to limited printing conditions due to the risk of thermal degradation [90, 91]. These works used transition state theory and DFT. They studied secondary reactions and defect structures, which may lead to thermal degradation or impact printed properties, comparing their likelihood and mechanistic favorability [85–88]. Reflecting the high computational cost of simulating large systems with quantum chemistry, they used minimal chains of a few repeating units.

Studies like those above that increase understanding of polymerization processes can help to explain and thereby optimize properties and printing conditions. Knowledge of defect generation may be incorporated into kinetic models to improve predictions of structure, and may be applied to developing stabilization approaches. However, quantum polymer rate constant studies suffer from a disconnect between theory and experiment for several reasons, including difficulty isolating individual experimental rate constants, difficulty accounting for full polymer chains with quantum chemistry, and large variations in accuracy of different quantum chemical methods. Lugo et al. [79] recently developed approaches to bridge this gap by mitigating errors associated with using minimal polymer fragments instead of full chains for DFT. They applied artificial strain to account for the reduced flexibility of mid-chain segments and incorporated explicit consideration of enantiomers to account for atacticity arising from chirality. For several acrylate secondary reaction types, this incomplete improvement, along with the inclusion of solvent effects (see Section 2.3), yielded better agreement with experimental rate constants than more traditional quantum approaches [79]. The authors then demonstrated the practical utility of such results by applying them alongside kinetic Monte Carlo techniques to predict chromatography traces, which can be used to describe printed gel systems.

Validation is important for striking the delicate balance between sufficient accuracy and sufficiently low computational cost in quantum chemistry. Computational setups must be tested to establish the applicability of molecular representations like minimal polymer chains, as well as methodological choices, such as the density functional and basis set. Computational results for selected systems covering relevant chemical space are compared to experimental data, with the above works using rate constant and activation energy data [85–88]. For DFT methods, different functionals and basis sets are compared to each other, as well as to more advanced wavefunction approaches [86, 88].

2.2.2 | Electronic Property Modeling

In addition to the reactivity of polymerizing systems, modeling can also aid with predicting and understanding properties of printed parts. Modeling electronic properties, such as the optical band gap of a polymer [52] or its electronically conducting or semiconducting nature [50], requires quantum chemical approaches. The utility of lighting or energy storage devices can be augmented using 3D printing of electronically active polymer inks, combining the precise spatial control of 3D printing with the desirable electronic properties of the polymer.

Yurkiv et al. [50] recently enhanced the electronic conductivity of a poly(3,4ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS)-based film for extrusion-based printing. They achieved this through tuning the ratio of the components, using dispersion-corrected plane wave basis set DFT calculations of band structure, density of states and mechanical properties to interpret their results. Yurkiv et al. [50] validated their choice of functional and basis set using known crystalline structures before applying the method to unknown amorphous ones. Similarly, Sun et al. [92] worked on developing 3D printable materials displaying room temperature phosphorescence for use in electronic devices. They used DFT to examine electron-donating capabilities of dopants for 3D printed matrices, explaining the mechanisms of the phosphorescence that they conveyed to the 3D printed systems.

2.2.3 | Simulating Realistic Conditions

The computational cost of quantum chemistry modeling can be prohibitive. Cost limits not only the size of systems that can be studied, but also accessible simulation conditions. As a standard, quantum chemistry studies are gas phase, static, and zero temperature (although quantum chemistry can be used in dynamic studies [93, 94], which comes at high computational cost). Successful 3D printing of polymers requires understanding processing conditions beyond the gas phase model and their impact on properties. In particular, interactions of monomers and polymers with solvent can inform the feasibility of formulation mixtures.

Solvation models are routinely used to account for chemical environment, extending the application space of quantum chemistry [95]. Interactions of explicitly described monomers or polymers with their solvent environment can be determined

to some approximation without expensive explicit inclusion of solvent molecules or with only some solvent molecules treated explicitly. Several implicit solvation models are available and may be applied to polymer studies, including the Polarisable Continuum Model (PCM) [96], Poisson Boltzmann (PB) implicit solvents [97, 98], and the COnductorlike Screening MOdel (COSMO) [99], a popular dielectric continuum model. COSMO was used to account for solvent effects in the acrylate DFT modeling of Lugo et al. [79], contributing to strong agreement with experimental rate constants (see Section 2.2).

An extension of the COSMO model, COSMO for Real Solvents (COSMO- RS) [43, 69, 71, 100, 101] gives relatively computationally cheap thermodynamic information using a small number of expensive quantum calculations of individual molecules and avoiding lengthy statistical sampling. Reusable quantum electronic structure calculations are performed once for all solvent and solute molecules, followed by fast calculation of electrostatic interactions [43] and additional contributions [101] (e.g., van der Waals interactions or hydrogen bonding) in a mixture. The chemical potential of a molecule in an arbitrary solution can be obtained and used to thermodynamically describe the system. It is possible to account for multiple conformers using COSMORS, with quantum calculations performed for each conformer [102]. This is valuable because COSMO-RS uses static representations of molecules, so conformations are not explored naturally.

Knowledge of solubility obtained from such solvation models has been used to inform polymer processes [28, 103]. and may be applied to 3D printable formulation design in terms of understanding the mutual affinity of formulation components before or after printing, covering monomers, pre-polymers and polymers, photoinitiators and photoabsorbers, and any solvent. There are multiple methods for solubility prediction, including empirical Hansen [104] and Hildebrand [105] solubility parameters [106] and machine learning models [107]. COSMO-RS is popular thanks to its versatility and the accuracy and detail it derives from quantum chemistry. It has been widely used [28, 108, 109] to guide solvent selection via prediction of monomer solubility in a range of media. In the context of 3D printing formulations, Zumaya et al. [110] recently demonstrated the use of COSMO-RS phase diagram and solubility calculations to examine the compatibility of poly(lactide), plasticizer additives and pharmaceutical molecules in 3D printed dosage forms. Their predictions were used to identify and explain optimal combinations of components. Use of similar approaches more widely in ink selection is an attractive prospect; for example, lignin is a promising sustainable, abundant, non-toxic biopolymer, amenable to 3D printing under the correct circumstances [111], but challenging to print because of low solubility [112]. Computationally screening formulation compositions to maximize solubility could expedite its widespread adoption in industry.

When including polymers in COSMO-RS calculations, adjustments and approximations are necessary to account for their size. Where there is a high degree of polymerization, it is common to use representative oligomers in place of long-chain polymers [28, 113]. COSMO-RS lends itself to an adaptation which allows these oligomers to better represent the polymers. As in the work of Zumaya et al. [110], the quantum calculation can be performed for a molecule, and then the charge distribution from the center of the molecule (the unit that repeats in the polymer) can be taken for further calculations and scaled based on polymer size. This adaptation will not, however capture all of the intra-chain interactions to fully describe the polymer. Additionally, free volume effects must be accounted for using an alteration of the COSMO-RS equations [113]. Meanwhile, there are specific aspects of polymer behavior relevant to 3D printing which are not readily addressed by COSMO-RS or similar approaches. Swelling and cross-linking are not easily captured [113], complicating modeling of parts post-printing.

2.3 | Force Field Simulations

Obtaining in-depth, time-resolved, chemical information involves statistical sampling methods, requiring energy evaluations at several timesteps. They are often paired with faster alternatives to costly quantum energy evaluation, especially for polymer systems which can contain several thousand atoms and above. Force field models are based on fitting some function of atomic positions to experimental or quantum chemical data of known systems, then transferring that function to evaluate energy and properties of unknown systems. Several relevant monomer and polymer properties tend to be predicted with force field methods, including viscosity, which can dictate printing feasibility and efficiency [40], and gel point, which informs post-printing properties [114].

Selecting an appropriate force field for a 3D printing study requires assessment of available models and the problems to which they may be applied. Force field simulations rely on appropriately selected methods and molecular representation, including atomic parameters and charges. Available force fields often accurately reproduce selected properties within a certain area of chemical space but struggle with generalizability and transferability. Force fields maximizing generalizability are desirable, particularly for in silico screening, in which properties are not known a priori.

2.3.1 | Classical, Atomistic, Non-Reactive Force Fields

All-atom force fields are parameterized to fit pre-defined functional forms based on underlying interatomic interactions, with defined atom types and bonding environment, and may be considered to be the most standard approach. They maintain atomic detail, naturally accessing phenomena such as hydrogen bonding and atomic-level structural rearrangements. However, they may be restricted by a lack of flexibility of functional form. They exist as sets of parameters, which are assigned to atoms in a system based on bonding environment. Partial charges are also assigned to atoms to describe electrostatic interactions. A method for deriving charges must be chosen to suit the needs of the system [115, 116], and can be based on reproducing ab initio electronic structure information [117–119], ab initio properties, or experimental data [120]. Recently, ML approaches for assigning atomic charges have been developed [121]. Multiple works have compared general atomistic force fields and their ability to reproduce specific experimental properties [45, 122, 123], demonstrating the dependence of performance on the problem at hand and highlighting the importance of validation.

Common force fields include the Generalized Amber Force Field (GAFF, now in its second iteration, GAFF2) [53, 124], which is a transferable choice applied widely, including for polymer chain molecules [123] and 3D printed systems. Gholami et al. [125] used GAFF2 to model rheological and ion transport properties of partially cured polymer composites with a view to predictive simulation for rational design. Other popular choices include the Chemistry at Harvard Molecular Mechanics (CHARMM) force field [54], and the all-atom Optimized Potentials for Liquid Simulations (OPLSAA) force field [126]. CHARMM, for example, was used by Koh et al. to explain printability and humidity resistance of a 3D printable bio-based cellulose hydroplastic [127]. Alternatively, more specific force fields may be used, such as the Interface Force Field, parameterized for organic–inorganic interfaces [128] and used by Gooneie et al. [129] to study polymer-metal interactions and conclude that a polymer of interest, polypropylene, may be used as a scaffold in metallic printing. Although these force fields are significantly computationally cheaper than quantum methods, using them to model polymers still requires specific considerations, such as use of short to mediumlength oligomers in place of full polymer chains. The polymer-metal interface work of Gooneie et al. [129] modeled 50-monomer chains, more units than quantum chemistry could access, but fewer than in a real sample.

Assignment of force field parameters involves specific challenges when polymers are involved. Practically, available structure files describing polymers may not contain sufficient information for automatic assignment [130], and chemical size and complexity can preclude manual assignment. Parameters may be assigned based on known topology of residues, particularly in well-defined systems. Automatic guesses of missing information may be used [131, 132], but available guessing methods are not always accurate. In a recent example aiming to address these challenges, Davel et al. [130] proposed a method within the Open Force Field [133] framework to parameterize polymer systems. They automatically matched molecular graphs of monomer templates to parts of the polymer graph. Assignment of partial charges in polymer systems is also not trivial. Polymer charges are usually explicitly derived for a monomeric unit and assigned in the polymer chain based on environment, reducing computational cost by reducing the size of quantum charge assignment calculations [134]. Davel et al. [130] used a formalized version of this approach. They also used an alternative approach based on ML for perceiving chemical environments in polymers.

Viscosity is a particular property amenable to force field prediction with wide relevance in 3D printing formulation design, and measures resistance to flow due to internal intermolecular interactions. Printing inks tend follow non-Newtonian and shear thinning behavior, illustrated in Figure 3a, in which viscosity decreases with increasing shear rate. Extrusion inks experience a range of shear stresses during printing. Their yield stress and shear-thinning viscosity response are critical in determining whether ink is released at a usable and controllable pace [40]. Meanwhile, light-based printing relies on ink coating a build plate, which is hampered by excessively high viscosity [135]. It is, therefore, important to know the viscosity of proposed inks, including on a high-throughput screening level. This applies particularly to pre-polymerized ink, ranging from small monomers to much larger oligomers: modeling entire network structures is not critical, but techniques relating to large molecules remain relevant.

Approaches to obtain viscosity predictions from MD and force fields can be separated into equilibrium and non-equilibrium methods. David et al. [27] used approaches of both kinds in studying the short polymer liquid n-hexadecane. They used the OPLS all-atom model refined for long-chain hydrocarbons (L-OPLS-AA) [136], along with examples of coarse-grained and reactive force fields (see Sections 2.3.2 and 2.3.3). In terms of equilibrium approaches, they used the Green-Kubo (GK) method [137] and the Einstein equation [138]. The GK method involves obtaining viscosity in the limit of zero shear from the plateau of a running integral of the autocorrelation function of pressure tensor components. Autocorrelation functions require long MD trajectories, but statistical noise is large at long integration times, and different trajectories of the same system differ significantly. Identifying the plateau region among this noise is challenging, and Zhang, Otani and Maginn [139] provided an automatable GK approach involving averaging over multiple independent trajectories to reduce noise, improve reliability and reduce reliance on human judgment. Figure 3b illustrates the GK method, including trajectory averaging.

David et al. [27] also applied a non-equilibrium approach, imposing a range of shear forces on n-hexadecane systems under the SLLOD equations of motion (named for their similarity to a method based on Doll's tensor) [140, 141]. Via the time-averaged response of the stress tensor, which describes the momentum flux, they obtained curves of viscosity against shear rate [27]. The SLLOD method allows granular analysis of shear-dependent viscosity behavior, as well as quantitative extrapolation to zero shear by fitting to an appropriate functional form. Fittings include the Carreau function as used by David et al. [27] or the Eyring equation used elsewhere [142]. Outcomes of the work of David et al. [27] include establishing the applicability of viscosity methods in the context of polymeric molecules, such that they may be considered applicable to screening 3D printable formulations. The authors compared force fields, finding that L-OPLS-AA is a strong choice in terms of experimental agreement for n-hexadecane, but suffers from high computational cost, necessitating alternative cost-reducing force fields for larger systems (see for example, Section 2.3.2).

Selection of viscosity simulation methods depends on the information required. Shear-dependent SLLOD curves are particularly instructive in the context of extrusion-based 3D printing methods, in which ink experiences different shear rates at different stages of the process. Zhao et al. [143] recently used non-equilibrium dynamics along with an all-atom force field to model shear-thinning behavior of a selection of binder polymer systems for alumina printing. They modeled viscosity and identified structural and bonding origins of shear thinning over the extrusion printing process. Such non-equilibrium methods can, at reasonably low computational cost, obtain predictions for viscosity at high shear. On the other hand, as highlighted in the work of David et al. [27], the computational cost of these methods is high if aiming to obtain accurate zero-shear viscosity. This may influence method selection where shear-dependent behavior is not critical. Meanwhile, the GK equilibrium method performs well for relatively low viscosity systems, but cannot

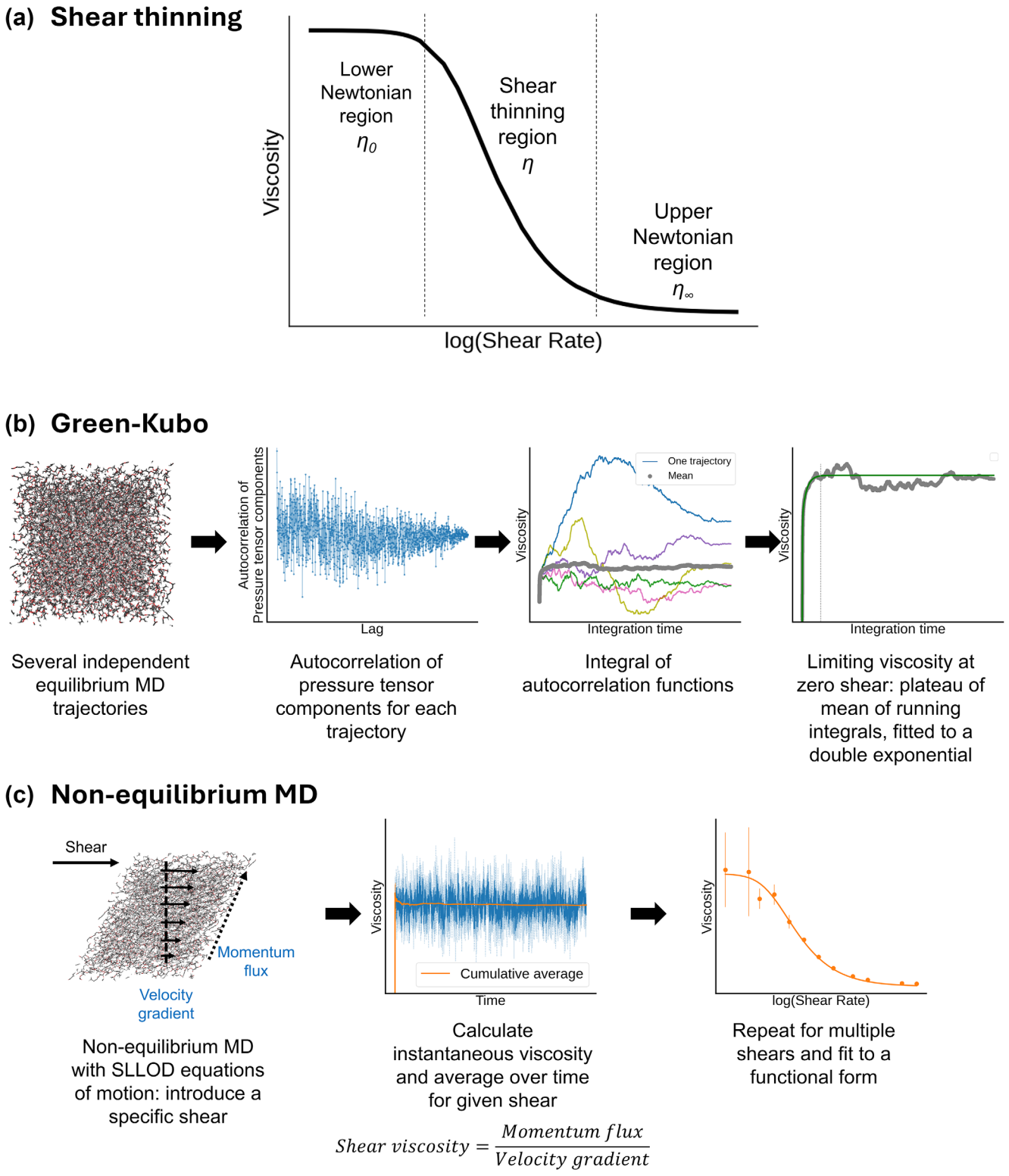

FIGURE 3 | (a) Illustration of the typical shear thinning behavior of polymer systems. (b) Illustration of the Green-Kubo method for calculating zero-shear viscosity using equilibrium MD, including trajectory averaging. (c) Illustration of viscosity calculations at specified shear using non-equilibrium MD and the SLLOD equations of motion.

readily be applied to high viscosity systems [144]. Completing long enough trajectories that the running integral adequately plateaus before excessive statistical noise obfuscates results is prohibitively expensive, particularly considering the necessity of several trajectories. Overall, viscosity simulation methods may be very useful under the correct circumstances, but tend to be characterized by difficulties associated with computational cost. In some cases, reducing computational cost by either enhanced sampling [144], modified force fields, or cheap heuristics, may be expedient.

2.3.2 | Coarse Graining

The distinctive physical properties of polymers, crucial for their applications in 3D printing, originate from their dynamical behavior across wide length and time scales [145]. All-atom (AA) MD simulations, while providing detailed chemical insight, are computationally expensive [146]. This limits their ability to access the long time and large length scales required to study many relevant phenomena in polymers, particularly viscoelasticity and entanglement dynamics. To overcome these limitations, a hierarchy of modeling approaches is employed, progressively reducing the system's degrees of freedom and increasing the simulation timestep [147].

One straightforward approach to increase computational efficiency while retaining atomistic detail is to use the SHAKE algorithm [148], which constrains high-frequency bond and angle vibrations, particularly those involving hydrogen atoms. This allows for a larger integration timestep (typically to 1–2 femtoseconds), enabling longer simulations [149]. Going a step further, united-atom (UA) models eliminate high-frequency hydrogen motions by merging hydrogen atoms with their bonded heavy atoms into a single interaction site, thereby increasing efficiency compared to explicit atom models [150, 151].

Coarse-grained (CG) models provide a more significant reduction in computational cost by grouping multiple atoms into a single low-resolution bead. This drastically reduces the number of particles to compute and simplifies interaction potentials, leading to a smoother energy landscape and enabling much larger integration timesteps, ranging from 5 to 20 femtoseconds for general CG models, allowing the exploration of longer timescales (up to microseconds) and larger system sizes (up to 10–100 nm) [147, 152, 153]. The atomistic details lost during coarse-graining can be partially restored through back-mapping techniques [154]. Several recent reviews provide comprehensive overviews of state-of-the-art methods for developing CG models for polymer studies [146, 155, 156].

Finally, slip-spring (SS) models represent an even lower level of resolution, using soft-core particles but crucially reintroducing topological constraints (entanglements) that are otherwise lost due to the soft potentials, thus enabling the correct prediction of entangled dynamics and rheological properties [157]. These highly coarse-grained models can access exceptionally long timescales, ranging from microseconds to milliseconds [158, 159].

One of the most important CG frameworks is the MARTINI model [160]. Initially developed for simulating biomolecular systems, the Martini force field has found broad application in soft material science. The Martini force field has a wide and expanding library of polymer models, with over 50 distinct polymers currently available [161].

CG models are powerful tools for screening various polymers and formulations relevant to additive manufacturing. The accurate calculation of polymer viscosity is a primary application of CG simulations for 3D printing, with various models and methodologies yielding distinct levels of success [157, 158, 162–167].

Padding et al. [168, 169] developed a CG model of polyethylene that accurately reproduced experimental viscosities for a broad range of molecular weights by integrating the shear relaxation modulus, obtained through equilibrium MD simulations. Similarly, Lemarchand et al. [164] developed a CG model for cis- and trans-polybutadiene showing 18%–50% agreement with experimental viscosity. Their method include applying the Irving–Kirkwood formalism to integrate pressure tensor data from the MD simulation (See Section 2.3.1).

A central challenge in using CG models for quantitative predictions is their inherently accelerated dynamics. The smoother energy landscapes of CG models lead to faster diffusion and chain motion compared to their AA counterparts. To accurately calculate physical properties like viscosity, this discrepancy must be resolved through a time-rescaling or corrections in the simulation's dynamics. For example, Khot et al. [165] reported UA and CG models for polydimethylsiloxane (PDMS) that could accurately reproduce experimental and AA-MD derived viscosity, after rescaling the time of the UA model by the factor of 2 and the CG model by the factor of 6, which was found in agreement with the previous studies of coarse grained polymer dynamics [170]. While time-rescaling is a common technique employed in CG studies, it generally doesn't allow for transferability of predictions across a broad range of temperatures [146].

A different approach includes modifying the system's underlying dynamics. Johnson and Phelan [166] developed a coarse-grained modeling strategy using iterative Boltzmann inversion (IBI). They introduced a tunable friction parameter to compensate for the accelerated CG dynamics, calibrating it to match the system's zero-shear viscosity, as calculated by the Green-Kubo (GK) method. For squalane, this approach successfully reproduced viscosities from AA simulations across a broad temperature range. They also highlighted a limitation in applying the GK method for longer chains, as the rise to a plateau viscosity can be very slow, exceeding practical simulation durations. A different approach was undertaken by Song et al. [171], they presented an energy renormalization (ER) strategy to develop temperature-transferable CG models for polymers, focusing on frequency-dependent viscoelasticity. Applied to polybutadiene (PB) and polystyrene (PS), their method involved renormalizing the cohesive interaction strength as a function of temperature and frequency to reproduce atomistic viscoelasticity. They reported reasonable agreement with both all-atom simulation results and earlier experimental measurements.

A multiscale modeling framework for polymers was reported by Liang et al. [157], linking all-atom, coarse-grained, and slip-spring models. They calculated the stress relaxation modulus using the Green-Kubo relation and then integrated it to estimate zero-shear viscosity, with subsequent time and modulus renormalization across scales. This approach achieved quantitative agreement with experimental measurements for the linear rheology of polystyrene. Similarly, Sgouros et al. [158] employed a hierarchical strategy for polyethylene, bridging MD to a slip-spring Brownian dynamics/kinetic Monte Carlo (BD/kMC) model. Their framework predicted the zero-shear viscosity in excellent agreement with MD and experimental data.

2.3.3 | Reactive Force Fields

In the context of polymers, simulating chemical reactions is crucial for understanding processes like polymerization and cross-linking that significantly influence material properties. The inherent approximations in potential energy descriptions in classical force fields limit their ability to model systems far from equilibrium, such as those involving transition states or chemical reactions.

Broadly speaking, there are two approaches to modeling reactivity in molecular dynamics. The first modifies classical force fields with reactive potentials, which account for changing attractions and repulsions based on the chemical environments within a covalent cutoff distance [172]. The second approach uses simple reactive rules in the MD algorithm, forming or breaking bonds when certain topology and energy requirements are met [173].

ReaxFF is the most popular reactive potential that also found applications in studying polymerization reactions. Vashisth et al. [49] used accelerated ReaxFF simulations to study reactive cross-linking of various polymer-forming epoxides. The force field was validated by successfully reproducing the energies and geometries of three possible transition states of the polymerization reaction. The cross-linking of diglycidyl ether of bisphenol F (bis F) and diethyltoluenediamine (DETDA) were studied with this method, achieving 82% cross-linking. Density, glass transition temperature and modulus of the simulated cross-linked polymer were found to be in good agreement with experiments.

Recently, Huang et al. [174] presented a modified ReaxFF force field for modeling of acrylate polymerization, another type of polymer widely used in 3D printing. The force field was also able to successfully reproduce densities and diffusion coefficients of the simulated polymers.

An alternative approach is the recently introduced reactive INTERFACE Force Field (IFF-R) [175], which models reactivity by replacing classical harmonic bond potentials with energy-conserving Morse potentials. Compatible with force fields such as CHARMM [54], OPLS-AA [126] and AMBER [53, 124], IFF-R enables bond dissociation by introducing three Morse parameters per bond type and zero energy upon disconnect. It was able to correctly reproduce mass density, elastic properties, yield strength, glass transition temperature, and thermal expansivity for various epoxy resins [176].

While bond-order potentials can provide valuable insights into transition energies, transition-state geometries, and reaction dynamics, their primary limitation lies in their high computational cost, which increases dramatically because of iterative charge equilibration and increased potential complexity [172]. In cases where reaction energetic details are not important, simpler methods can be used. These methods model the reaction with simple cutoff rules, creating bonds between atoms that match predetermined topology and conditions (distance and energy) [173, 177]. Although it cannot properly describe reacting energies and dynamics, this approach allows very fast modeling of chemical reactions at the same cost as classical MD and has been widely used for polymerization studies [178–180].

In the context of 3D printing, the gel point is particularly important because it determines the degree of polymerization or cross-linking required for a material to transition into a gel. Accurately modeling gel point involves exploring a broad range of molecular weights and cross-linking degrees, making a reactive MD approach based on simple cutoff rules a convenient and efficient choice. Torres-Knoop et al. [178] studied the free-radical polymerization of hexanediol diacrylate, determining the gel point and successfully reproducing glass transition temperature and Young's modulus at conversion close to the experimental value. Monteferrante et al. [181] studied polymerization of 1,6-hexanediol dimethacrylate systems for different concentrations of radicals and characterized the obtained polymers in terms of viscosity and diffusion constant, in addition to gel point. Livraghi et al. [182] developed a systematic block approach to modeling of epoxy resins; by deriving the charges and defining the reactivity of predefined building blocks, the method was shown to reproduce experimental gel points well.

2.3.4 | Machine Learning Force Fields

Machine learning-based force fields (ML-FFs) aim to bridge the gap between the computational efficiency of classical force fields and the accuracy of quantum methods. In contrast to classical approaches, ML-FFs do not rely on predefined functional forms or fixed chemical connectivity. Instead, they employ machine learning models to learn the complex relationship between atomic coordinates and the system's potential energy. In principle, the predictive accuracy of ML-FFs is limited only by the amount and quality of their training data and the underlying machine learning algorithm [183].

The main challenges in constructing ML-FFs are scalability and generalizability to systems outside of the training set. A significant hurdle in developing robust ML-FFs for polymers is extrapolating from computationally feasible training data, typically derived from high-level quantum calculations on monomers and short oligomers, to accurately predict the behavior of large-scale, bulk polymer systems.

ML-FFs have shown considerable promise for the prediction of polymer properties [184]. For instance, Mohanty et al. developed a charge recursive neural network (QRNN) that successfully generalized from small training clusters to predict properties of ethylene glycol oligomers [185]. While the model underestimated the density of polyethylene glycol by approximately 5%, it demonstrated superior performance compared to OPLS4 FF in capturing properties such as self-diffusivity and heat capacity. ML-FFs have also proven to be effective for predicting the mechanical properties of polymers. Hong et al. developed an ML-FF for polytetrafluoroethylene (PTFE) using a Gaussian process regression model [186]. Their potential was highly effective in predicting the material's Young's modulus, demonstrating an error margin of less than 2% compared to experimental values.

More recently, the PhyNEO framework introduced by Chen and Yu combines physics-informed and data-driven strategies to parameterize polymer force fields [183]. By training exclusively on quantum mechanical data from small molecular fragments, their model demonstrated superior accuracy in predicting the

bulk densities of poly(ethylene oxide) and polyethylene glycol when compared to established classical force fields like GAFF and OPLS.

Another innovative approach is the PolyGET framework [187], which utilizes generalized equivariant transformers. This model is notable for its strategy of optimizing forces directly, rather than jointly optimizing energy and force, and has achieved state-of-the-art accuracy and computational speed across a diverse dataset of 24 different polymer types. While the framework shows great potential for generalizability, its application to the prediction of bulk polymer properties remains an area for future exploration.

3 | Data-Driven Polymer Discovery

Traditional polymer design for targeted applications often involves multiple iterative refinements, with insights gained from addressing failures [188, 189]. However, trial-and-error strategies can restrict innovation due to constrained design space and reliance on chance discovery [189, 190]. To overcome these constraints, high-throughput experiments, virtual screening, and physics-based modeling, as discussed in earlier sections, now enable more systematic and predictive assessment of properties [191].

Nevertheless, despite advancements in high-throughput simulations and GPU-accelerated technology, the complex demands of polymer discovery often outpace current methods [192]. Here, machine learning (ML) and artificial intelligence (AI) have emerged as essential tools in conjunction with physics-based simulation methods and in their own right, transforming polymer design by efficiently mapping complex structure–property relationships to predict desired features and recommend optimal experimental conditions, given sufficient and high-quality data [14, 187, 193–196]. This shift enables a more targeted approach, facilitating rapid exploration of vast chemical spaces and enhancing the precision of predictive modeling [197, 198], particularly in the development of quantitative structure–property relationship (QSPR) models [194, 199–202]. Figure 4 outlines the typical ML/AI-assisted polymer discovery pipeline. The process begins with data collection from published literature and existing databases, complemented by data generation through experimental and computational methods. Following data preprocessing steps, such as data cleaning and normalization, the most relevant polymer information is extracted and utilized as input for ML/AI models. These models generate predictive insights that guide polymer characterization and materials design, with appropriate algorithms selected based on the specific application. The predicted results, along with a well-established surrogate model, contribute to expanding the chemical design space and are integrated into databases, enabling iterative optimization of polymer properties. Feedback loops between ML/AI models and experimental/computational validation further enhance data augmentation and accelerate the discovery and development of novel polymeric materials.

3.1 | Data Sources and Preparation

Advancements in data-driven research are contingent upon organized, accurate and clean data [203], following the findable, accessible, interoperable, and reusable (FAIR) principles [204] for data storage and management [205]. Gathering data from existing literature is a commonly employed approach, valued for its efficiency in both time and cost [206]. Additionally, the advancement of large language models (LLMs) and their associated algorithms has significantly enhanced the data mining process, showing high reliability. However, data obtained from such resources may exhibit inaccuracies and a deficiency in critical contextual metadata, which is essential for the effective aggregation and comparison of datasets across diverse sources or authors. In addition to journal publications, there are classic handbooks encompassing foundational knowledge on polymers, including chemical structures, properties, and methods of synthesis [207–213]. Recently, a variety of polymer databases have been digitized, providing streamlined access to comprehensive polymer data, for example, PoLyInfo [214], CHEMnetBASE-Polymers [215], and Polymer Genome [216]. However, some remain inaccessible to the public [217]. Most contain empirical data, owing to the high computational complexity involved in

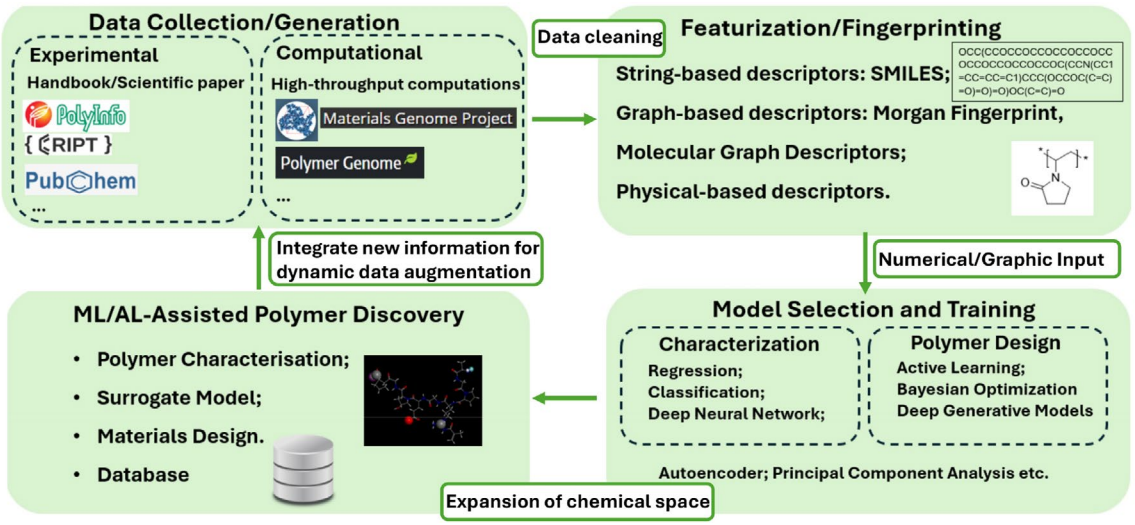

FIGURE 4 | Pipeline of ML/AI-assisted polymer discovery.

simulating polymers [218], but simulation data can also play a part in polymer ML work [219]. Table 1 summarizes commonly used methods for obtaining polymer data along with operational requirements and other considerations.

Compared to data mining, generating in-house data offers more precise control over experimental conditions and facilitates the exploration of novel materials. Nevertheless, in data-driven studies, a substantial data volume is typically regarded as crucial, especially for training deep learning models. Due to the complexity and high costs associated with experimental data collection, it is uncommon to amass thousands of in-house polymer samples under uniform conditions. A design of experiments (DoE) approach can be used to maximize the amount of information gained for an effective ML implementation from a pilot set of materials [220].

Physics-based simulations can also play a powerful role in conjunction with data-driven techniques. Robust computational data sets can be an alternative to both data mining and in-house experimental data [194, 219]. For example, Choi et al. [221] trained neural networks to predict glass transition temperature (Tg) and other properties of cured epoxy resins as calculated from the results of reactive MD simulations. Integration of MD and ML enables automatic detection of changes in resin components, streamlining the screening process compared to traditional trial-and-error methods. Vassileiou et al. [222] used COSMO-RS predicted solubilities as descriptors to inform the prediction of experimental solubilities for organic systems and found an improvement compared to models trained without simulation data. Using simulation data as ML targets in this way can circumvent many difficulties relating to experimental data: compared to experiments, computational methods involve more easily standardized conditions and data are often more efficiently generated. Meanwhile, rather than using physics-based simulation data as an input feature directly, Xu et al. [223] developed SLIMNet, a neural network model based on scaling laws that modifies the output layer to predict undetermined parameters. By incorporating physicochemical prior knowledge, the model enhances performance through subsequent computations. However, as discussed in earlier sections, computational polymer simulations present other challenges relating to the size and complexity of polymers and the trade-off between computational cost and accuracy.

Apart from optimizing input data and model integration, employing an appropriate ML framework can enhance simulation accuracy inexpensively [224]. While larger datasets have the potential to improve model performance for certain algorithms and applications, the literature provides examples of successful ML implementation with significantly smaller datasets, as few as 43 polymers to several hundred [225–227]. Selecting a machine learning algorithm is closely linked to the volume of available data, as certain model algorithms can achieve high performance even with smaller datasets. The specific ML/AI applications in polymeric materials will be discussed in detail in Sections 3.3–3.5.

3.2 | Polymer Informatics

Accurate and precise representation of polymers is essential for achieving robust predictive accuracy [228]. Polymer informatics aims to identify patterns within extensive datasets of existing or generated polymer information to enable the design of new functional polymers. The optimal selection of polymer representation varies depending on the property to be predicted, input data type, and ML approach.

The simplified molecular input line entry system (SMILES) is one of the most widely used line notations for representing molecular structures. It was developed to efficiently encode chemical information in a machine-readable format [229]. As an extension to SMILES, BigSMILES is a modification for polymers to represent the structural units [230]. However, due to the undefined number of repeating units and structural complexity, properly encoding polymers with BigSMILES as a discrete input remains a significant challenge [231]. In addition to BigSMILES, PSMILES extends conventional SMILES to represent stochastic polymer structures, including homopolymers and copolymers. It supports encoding connection variability and can be transformed into PolyBERT [232] input for deep learning models

TABLE 1 | Methods for obtaining polymer data.

Method	Operation	Consideration
Literature mining	Manual or automated text-mining tools	Additional curation to ensure consistency and completeness.
High-throughput experiments	Custom hardware and specialized skill set	Time-consuming and costly; Standardization required; Mostly available for non-novel polymers.
High-throughput simulations	Specialized skill sets: molecular dynamics (MD), density functional theory (DFT), and finite element analysis (FEA)	Computational expense; High quality input dependent; Experimental validation is required.
Curated databases	May collect data manually (no application programming interface (API) available)	Limited data type and size (only specific properties and unavailable metadata); Heterogeneous data.
Synthetic data generation	Well-established computational model	Training data dependent; Bias or errors in various cases.

or into molecular descriptors for traditional ML workflows. However, complex copolymers, such as gradient copolymers, cannot be displayed easily by PSMILES [233].

For deep learning applications, there is potential to tokenise BigSMILES as text for LLMs or to treat it as an image input for graph neural networks (GNNs) using kernel methods [234]. However, supporting evidence in the literature is still limited. Very recently, Qiu et al. [235] evaluated the performance of SMILES and BigSMILES, by employing the image representation of BigSMILES as the input of convolutional neural network (CNN), meanwhile tokenizing BigSMILES for LLMs. BigSMILES enhanced training efficiency by offering a more compact and structured representation of complex polymer architectures than conventional SMILES. As an extension of BigSMILES, G-BigSMILES is another notation method that incorporates reactivity ratios, molecular weight distributions, and ensemble size, streamlining the representation of complex polymer ensembles [231]. Tran et al. [236] comprehensively reviewed notable polymer informatics platforms, with a focus on AI-driven polymer design for diverse applications.

The most common strategy is to capture polymer key features, for example, constitutional unit or functional group, from a SMILES representation [198, 218, 228, 237–240]. This strategy, rooted in the early "group contribution" methods, marks the origin of polymer informatics [241]. The numerical representation of these "units" or "groups" can be encoded using various descriptor or fingerprinting methods, serving as a standard input for classical ML/AI models. One-hot encoding (OHE) is a simple approach that is commonly used to represent categorical variables. When used as a polymer fingerprint, OHE is limited to identifying constitutional units without conveying chemical similarity [242]. In contrast, Morgan fingerprints, among the most widely utilized molecular descriptors, encode connectivity and atom features in all substructures within a defined radius [243, 244]. Beyond these, several descriptor engines offer richer numerical representations [245]. Mordred is a comprehensive descriptor generator capable of calculating over 1800 2D and 3D descriptors [246], including topological indices, geometrical properties, constitutional features, and physicochemical parameters. This allows it to capture both the structural layout and spatial characteristics of molecules. RDKit is an open-source cheminformatics toolkit [247], that provides a robust set of primarily 2D descriptors, such as molecular weight, logP, polar surface area, and counts of specific functional groups. As a commercial software package, Dragon can calculate over 5000 molecular descriptors spanning from 0D to 3D, including constitutional, topological, geometrical, and electronic properties [248]. These advanced descriptor sets allow for more detailed and chemically meaningful representations, enhancing the predictive power of ML models in polymer informatics, and enabling more explainable approaches.

Depending on the dataset, fragment-level descriptors capturing polymer substructures have also been effectively used for ML training [228, 249]. Additionally, hierarchical framework fingerprints have been developed to encapsulate the connectivity and morphological characteristics of polymers, enhancing the accuracy of property prediction [216, 250–252]. The graphs extracted from the SMILES representations of oligomers can also be used as input to ML models, where nodes and edges represent atoms and bonds [253, 254]. The complex substructures and the high number of monomers present in polymers still present significant challenges in this context.

3.3 | Machine Learning/Artificial Intelligence Applications for Polymers

Based on the model supervision approach, machine learning is divided into supervised learning, unsupervised learning, and reinforcement learning. Supervised learning includes regression and classification tasks, where models are trained on input data paired with known "labels," that represent either the output values or target variables linked to the input. In contrast, unsupervised learning methods like clustering and dimensionality reduction operate on data without output labels, aiming to extract hidden patterns or structures. Reinforcement learning is an iterative approach under the active tutelage of an agent. Rather than learning from either static labels or purely unlabeled data, reinforcement learning performs actions to adjust its condition and interact

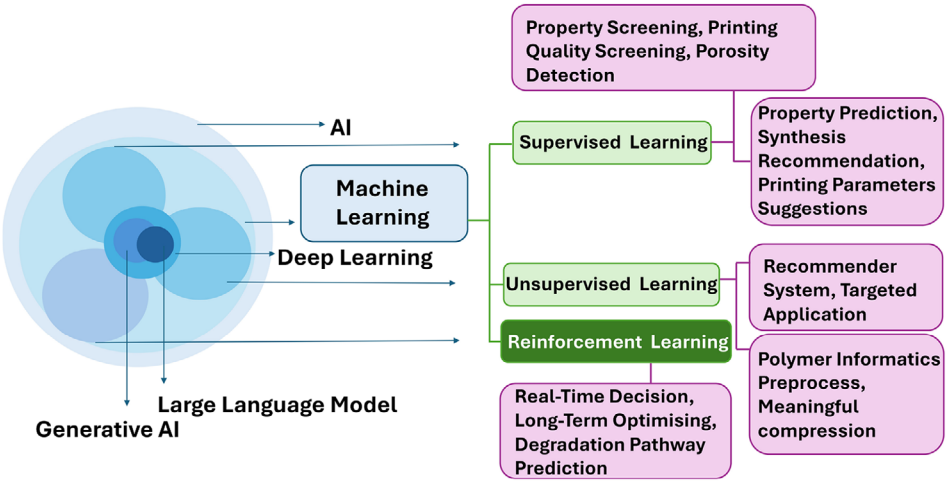

FIGURE 5 | Classification of artificial intelligence (AI), machine learning models and relevant applications in polymer research.

dynamically with the environment, aiming to maximize a designated reward value [255]. Figure 5 shows the classification of machine learning models. Different algorithms can be effectively applied in polymer discovery to address various application-specific tasks. A summary of the full pipeline to generate predictive outcomes is highlighted in Figure 6. Polymer information retrieved from the database undergoes processing contingent on the specific deep learning algorithm employed. Property prediction, structure generation, feature recognition, and functional group importance can be facilitated in different model applications. The generative model architecture will be illustrated in Figures 8 and 9.

An essential aspect of effective ML/AI implementation is robust feature selection, which ensures the input variables are both relevant and informative for the target property. Based on their relevance to the target property and potential redundancy, features can be grouped into irrelevant features, redundant features, weakly relevant but non-redundant features, and strongly relevant features [257, 258]. Beyond the careful selection of polymer representations discussed in Section 3.2, common strategies include feature engineering guided by chemical knowledge and automated methods. Automated methods include filter, wrapper, and embedded methods [259].

Filter methods apply simple statistical criteria to assess each feature independently of any model, offering computational efficiency but often ignoring feature interactions [260, 261]. Examples of filter methods include variance thresholding [262], correlation based ranking [263], mutual information scores [264], and Chi-squared tests [265], which all evaluate features independently of the predictive model [266].

In contrast, wrapper methods select features by explicitly searching for the subset that gives the best model performance. They do this by repeatedly training the model on different feature combinations and comparing results. Like recursive feature elimination, this approach iteratively refines and removes features based on model performance to find an optimal subset, although it can be computationally intensive [267–269].

By comparison, embedded methods integrate feature selection directly into the model training process itself. In this case, the model automatically either selects or weights features as it learns. For instance, tree-based algorithms determine feature importance through their splitting criteria, while regularization techniques such as LASSO shrink coefficient values toward zero to eliminate less relevant variables [270]. However, features with weak individual effects but strong relevance when combined with others may still be penalized or discarded by embedded methods, particularly those based on regularization [271]. Regularization-based models are a classic example of embedded methods, since they integrate feature selection directly into training by penalizing model complexity [272]. Examples including Ridge regression [273], LASSO [274], and Elastic Net [275], add penalty terms to the model's loss function to constrain coefficient magnitudes. This approach helps reduce model complexity and mitigates overfitting, which occurs when a model fits noise rather than capturing meaningful trends.

Moreover, to address overfitting, various cross-validation methods are widely employed depending on the case to assess model generalizability [276–280]. Common approaches include k-fold cross-validation [281], where the dataset is split into equal folds for iterative training and testing, and leave-one-out cross-validation (LOOCV) [282], which is particularly useful for small

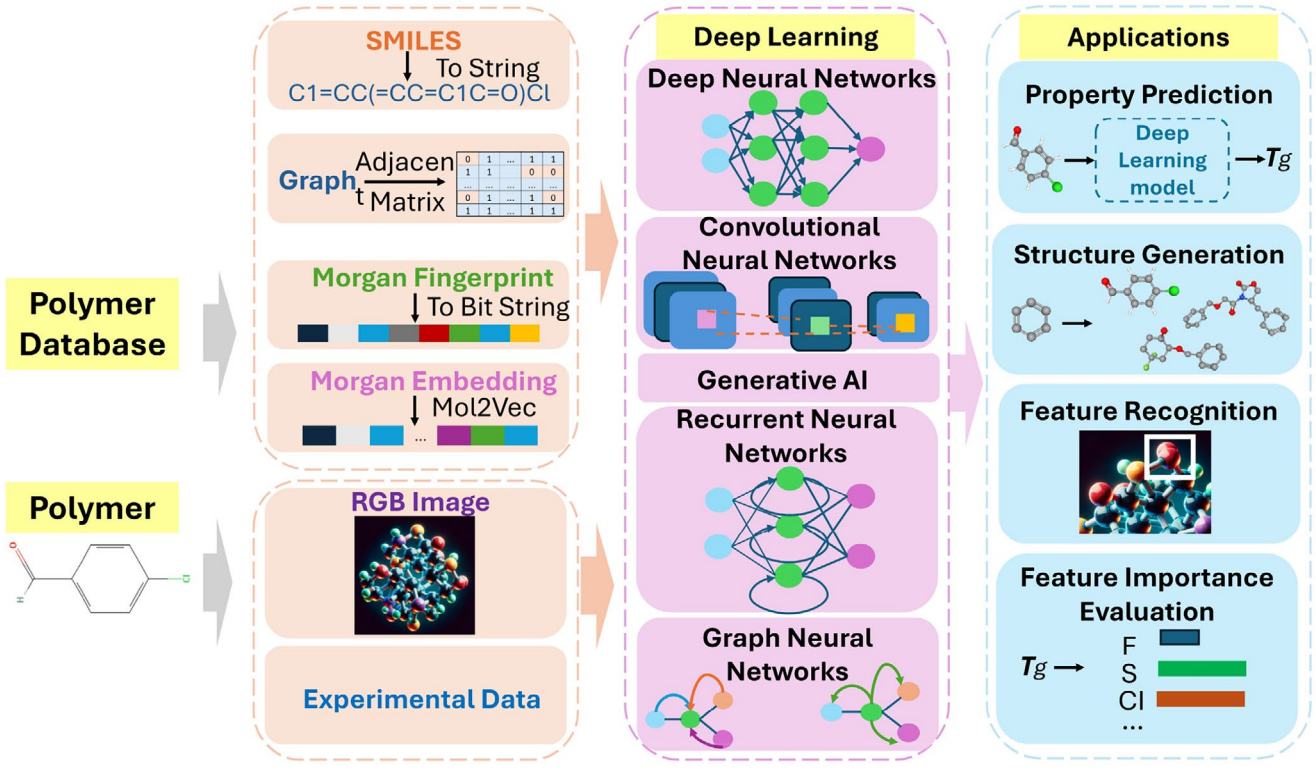

FIGURE 6 | Key aspects of deep learning applications in polymeric materials. Adapted from [256].

datasets. Stratified k-fold cross-validation is often applied when class imbalance must be maintained across folds [283, 284], while group k-fold, prevents data leakage by ensuring related samples appear only in the same fold [285]. For unbiased hyperparameter optimization, nested cross-validation combines an inner loop for model selection with an outer loop for final performance assessment [286]. Additionally, Monte Carlo cross-validation, which relies on repeated random subsampling, can provide flexible validation for imbalanced datasets [287]. Choosing an appropriate validation strategy depends on dataset characteristics, task requirements, and the need to control overfitting [288].

However, the generalizability of ML/AI models can be limited if the training data cover only a narrow range of polymer chemistries or specific 3D printing conditions. For instance, models developed for semi-crystalline thermoplastics used in FDM may not directly apply to crosslinked resins in vat photopolymerization processes such as SLA or digital light processing (DLP) without additional retraining or adjustment of input features [16, 289, 290]. Therefore, careful curation and diversification of training data help ensure that developed models are generalizable across a wider range of polymer chemistries and processing methods, including diverse 3D printing applications [291–293].

3.4 | Polymer Characterization

Regression-based modeling focuses on predicting numerical or quantitative outcomes, which can be used to predict polymer physicochemical properties relevant to AM, for instance, glass transition temperature [243, 294, 295], mechanical strength [296–298], viscosity [299–301], and degradation [302, 303]. Technically, logistic regression is a classification algorithm designed for binary classification problems. The categorical output typically is 0/1, Yes/No, or True/False. Classification-based models aim to identify and establish boundaries that distinguish between predefined categories, which are commonly used for polymer screening. Vaghefi et al. [304] compared different classification algorithms on the thermal response of poly(methyl methacrylate) (PMMA), aiming to differentiate pure PMMA from its composite through an intelligent, non-destructive method. Their methodology involved a feature extraction phase, utilizing data derived from mass measurements using a precise scale, cooling time, and the initial and final temperatures of each specimen as recorded by a thermal imager. Moreover, three distinct oversampling methodologies were implemented to address data imbalance and scarcity. This study highlighted the strength of ML for polymer screening, even in scenarios of limited data, making it particularly valuable for 3D-printable materials, where literature data remains scarce.

Before the emergence of generative AI, support vector machines (SVMs) were considered a classic technique for dealing with high-dimensional data like descriptors and fingerprints. They were widely applied in image recognition, text categorization, and bioinformatics [240, 305–308]. As introduced in Sections 3.2 and 3.3, feature selection is necessary when input dimensionality is as high as it is the case in polymer informatics. In contrast to keeping beneficial input features, principal component analysis (PCA) reduces redundancy by transforming the whole input dataset into uncorrelated principal components. By reducing the dataset dimensionality, the input space can be more efficient and this avoids duplication of information [309–311].

Other algorithms, including decision trees, random forests, neural networks, knearest neighbors, Gaussian processes, and gradient boosting, also demonstrate versatility, allowing them to be utilized effectively for classification and regression tasks. In polymer studies, multiple algorithms are often employed to conduct comparative analyses on the same research problems. For instance, Kumar et al. [312] compared linear and polynomial regressions with support vector regression (SVR), neural network (NN), and gradient boosting regression (GBR) for simulating the poly(2-oxazoline) cloud point. By considering computational cost, results accuracy, and complexity of hyperparameter tuning, specific algorithms are prioritized in different cases. Tao et al. [249] built a feed-forward neural network (FFNN) and gradient boosting machine (GBM) to simulate the fractional free volume of polymer membranes. The GMB model demonstrated superior performance across 123 microporous polymers, despite the great computational expense involved. In contrast, the FFNN model exhibited commendable performance in virtual screening of the fractional free volume of 8 million polyimides, following training on 80% of a dataset comprising 6500 homopolymers and 1400 polyamides. Moreover, various algorithms can be integrated to improve predictive accuracy and achieve more sophisticated outcomes. Methods using this approach are commonly referred to as ensemble-based methods [124, 313–316]. Given the multiple parameters involved in the polymeric 3D printing process, along with the inherent characteristics of polymers, it is crucial to implement integrated algorithms for reliable predictions [292, 317]. Khusheef et al. [318] proposed a hybrid CNN-long short-term memory (LSTM) architecture, using sensor signals and thermal images collected during printing along with printing parameters as input, enabling precise prediction of surface roughness, warpage, tensile strength, elongation at break, and micro-hardness of 3D printed polylactic acid. Gao et al. [196] designed an ensemble learning integrating k-nearest neighbors (KNNs), Gaussian regression, kernel ridge regression, RF, and artificial neural network algorithms in each sub-model, aggregated via LASSO regression. Hardness, tensile strength, and elongation at break of 3D printed photopolymers were predicted with high-precision.

Glass transition temperature is a crucial polymer property. It is widely discussed [209, 319] and can inform whether a candidate polymer is appropriate for a 3D printing application. In Table 2, we list recent ML/AI-assisted polymer characterizations for glass transition temperature prediction, including algorithms, data sources, and model input types. Apart from conditional tabular generative adversarial networks (CTGAN), which is a generative algorithm, the rest of the methodologies are applied to property prediction.

3.5 | Polymer Discovery

As generative models continue to evolve through emerging techniques, they are becoming powerful tools in polymer

TABLE 2 | Examples of ML/AI-assisted polymer characterizations for glass transition temperature simulation.

Methodology	Data source type	Informatics type	References
Least absolute shrinkage and selection operator (LASSO) Regression, deep neural network (DNN), and convolutional neural network (CNN)	Online database: PoLyInfo, PI1M	Molecular descriptors, Morgan fingerprints, and images	[243]
Ridge regression, artificial neural network (ANN), CNN	Online database: PolyInfo	Physicochemical descriptors, topological descriptors	[320]
Ordinary least squares (OLS) multiple linear regression	Scientific paper, in-house experiments, MD simulation	Manually selected molecular features	[321]
Graph convolutional neural network (GCNN)	Online database: PolyAskInG	Molecular graph	[322]
LSTM	Online database: SciGlass	One hot vector encoded SMILES	[323]
Locally linear embedding, eXtreme gradient boosting (XGB), Genetic algorithm (GA)	Polymer handbook	Molecular descriptors	[256]
Extra trees (ET)	Scientific paper, in-house experiments	Functional groups, and featurizer RDKit descriptors with melting temperature	[324]
Conditional tabular generative adversarial networks (CTGAN), ANN	Synthetic data from CTGAN, scientific paper	Curing condition	[325]
Gaussian Process Regression (GPR), Monte Carlo Dropout (MCD), meanvariance estimation (MVE), Bayesian Neural Network based on Variational Inference (BNN-VI) and Markov Chain Monte Carlo (BNN-MCMC), evidential deep learning (EDL), quantile regression (QR), natural gradient boosting (NGBoost)	Online database: PoLyInfo	Morgan fingerprint with frequency	[326]

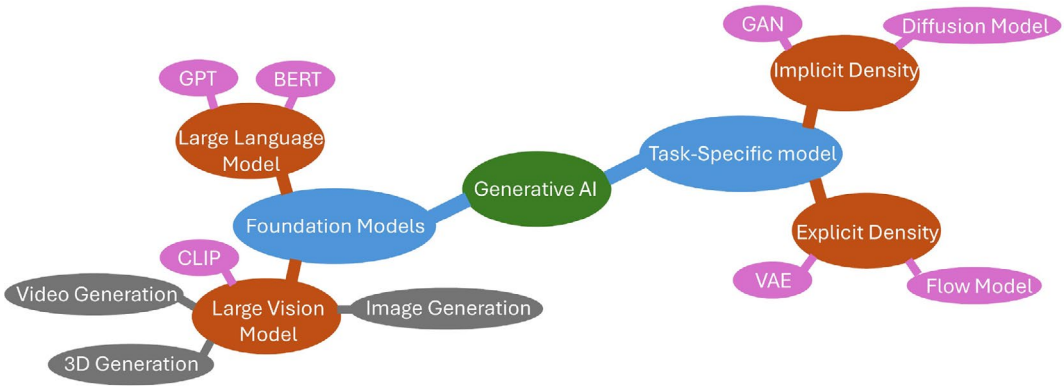

FIGURE 7 | Types of generative AI models with a focus on foundational models and task-specific models.

research, particularly in the discovery of novel materials with tailored properties [327, 328]. Figure 7 illustrates the various types of generative AI models. In the context of polymer discovery, these models can effectively learn the underlying distribution of chemical datasets and explore them to design polymers with desired characteristics [30, 314, 329, 330]. Consequently, generative AI extends beyond conventional property prediction or structure–property mapping; it can be used to generate entirely new molecular structures with targeted functionalities. This paradigm is commonly referred to as inverse design, especially when applied to identifying optimal synthesis pathways and processing parameters [331, 332]. The application of machine learning (ML) and deep learning (DL) techniques for the inverse design of polymers has been comprehensively reviewed by Sattari et al. [239] Both classes of generative AI models depicted in Figure 7 have been widely

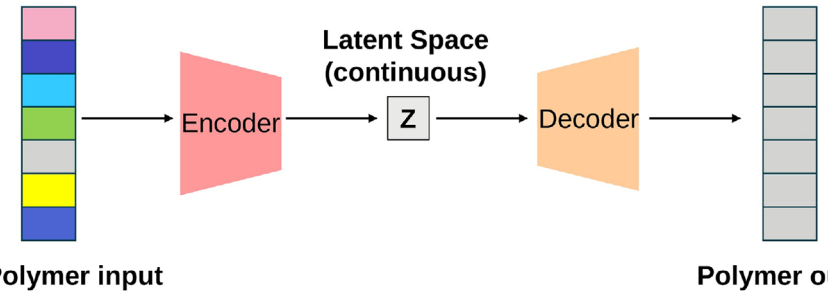

FIGURE 8 | Schematic illustration of the structure of VAEs. A defined polymer input is encoded to latent space, with decoding affording generative access to new polymers.

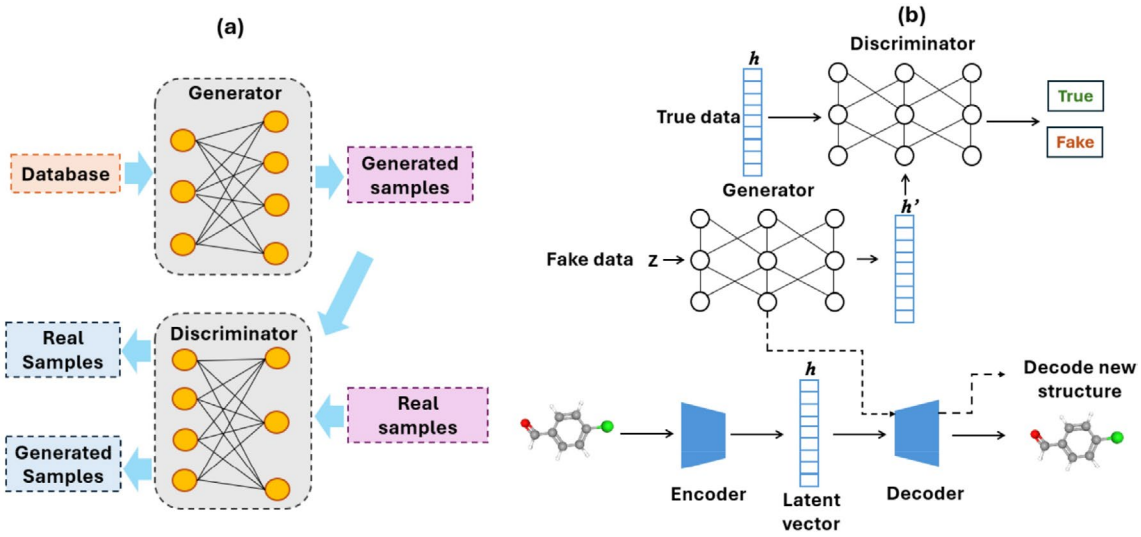

FIGURE 9 | (a) The fundamental architecture of GANs, consisting of a generator and discriminator. (b) The employment of GANs in generating molecular structure. Adapted from [256].

adopted in polymer science, supporting tasks ranging from information extraction and reprocessing to property prediction and the generation of novel polymer candidates. Recent advancements have also integrated rule-based polymerization reactions with generative approaches to construct large-scale databases of hypothetical polymers, greatly expanding the accessible design space. However, the complexity of polymer science, stemming from the structural diversity of polymers, the broad spectrum of their properties, and the scarcity of high-quality training data, are significant challenges yet to be overcome for developing accurate and generalizable predictive models [333].

In the following section, we introduce several of the most widely used generative AI techniques applied in polymer research.

Large language models (LLMs) present significant advancements in natural language processing (NLP), with prominent examples such as bidirectional encoder representations from transformers (BERT) [334, 335]. These models have revolutionized literature mining, enabling more efficient and accurate extraction and analysis of scientific information. LLMs are now widely applied in tasks such as database extraction [336–339], materials discovery [340–342], and large-scale information analysis [343, 344]. In polymer science, NLP has also been used to develop pipelines for extracting polymer property data [341].

BERT-like models can generate contextual text embeddings to gain unseen knowledge. These specialized BERT models are tailored to capture domain-specific characteristics. They include MechBERT extracting stress–strain properties [345], BioBERT for bio-medical data mining [346], as well as OpticalBERT [347], and BatteryBERT [348]. Kuenneth et al. [232] developed a chemical linguist, polyBERT, which enables an ultra-fast polymer informatics pipeline for property prediction. Similar work has been done by C. Xu et al. [349] with TransPolymer. More recently, Qiu et al. [350] proposed PolyNC, which can process both natural language and chemical language, by employing a text-to-text transfer transformer (T5) [232], an encoder-decoder model. These advancements in domain-specific language models demonstrate the power of NLP tools in capturing complex scientific relationships and accelerating data-driven discovery in polymer science. In parallel with these developments, generative models, especially variational autoencoders (VAEs) have emerged as foundational frameworks for molecular and material generation.

As early generative frameworks, VAEs utilize an encoder-decoder structure grounded in probabilistic graphical modeling to extract latent representations for output synthesis [351].

In polymer discovery, the data being processed can be either descriptors or graph-based representations. They are encoded into a lower-dimensional latent space using models like VAEs. While conceptually similar to dimensionality reduction techniques like PCA, VAE encoding is nonlinear and probabilistic, capturing more complex relationships. A decoder then reconstructs the polymer structure from this latent space, enabling the generation of novel polymers. Commonly, VAEs are coupled with predictive tools, for example, GPR [352], Bayesian optimization [353], or weighted-vector combination method (WVCM) [354]. The core architecture of VAEs designed for processing polymers is illustrated in Figure 8.

Since molecular generations can be viewed as probabilistic autoregressive processes, recurrent neural networks (RNNs), comprised of several interconnected layers of LSTM, have been trained as generative models for this purpose [355–357]. Moreover, RNNs are frequently applied to VAEs to build a hybrid deep encoder-decoder architecture [358–361]. With the VAE framework smoothing out the latent space and sampling more realistic results, RNNs leverage the strength in capturing temporal dependencies, which can be employed as either encoder or decoder [362, 363].

While RNNs and VAEs excel at sequence modeling and probabilistic latent space learning, generative adversarial networks (GANs) represent a fundamentally different paradigm, one based on adversarial training that has revolutionized generative AI. In this framework, a generator network attempts to create realistic samples, such as molecular structures or material images, while a discriminator network tries to distinguish between real and generated data. Through this adversarial process, the generator progressively improves, ultimately producing highly realistic outputs [364, 365]. This has led to major advances in materials discovery, enabling tasks such as inverse design, realistic sample generation, and data augmentation for low-resource domains [366]. Figure 9 depicts the basic structure of GANs and their application in molecular structure generation. Jabbar et al. [35] have reviewed a detailed classification of GANs. To achieve better performance, different architectures have been utilized in GAN models, for example, supervised regressor networks [367], and CNN [368–370]. Dong et al. [367] designed a regressional and conditional GAN (RCGAN) for the inverse design of graphene and boron-nitride (BN) hybrids. The integrated supervised regressor network facilitated data generation from continuous and quantitative labels, enabling the association of generated structures with target properties. Blarr et al. [371] proposed a deep convolutional GAN able to generate unlimited numbers of realistic CT images of microstructures of carbon fiber-reinforced polyamide. Notably, the fiber orientations and bundles were not reproduced but generated independently. Additionally, a plausible synthetic dataset can be generated by the GANs-based method to augment the limited available data, like conditional tabular GANs (CTGAN) [325, 372, 373], and conditional generative adversarial networks (CGAN) [374]. Wang et al. [325] developed a CTGAN-ANN framework, where an ANN was trained on the CTGAN-synthesized Tg data duplicated from experiments. This approach achieved an $R^2 \geq 0.95$ validated against real experimental data. Liu et al. [375] proposed a GAN-tree-based pipeline optimization tool (TPOT), where GAN was used to expand the original input dataset, while TPOT conducts automated regression ML for predicting Tg of solution styrenebutadiene rubber.

3.6 | Extended Use of AI and ML in 3D Printing

The integration of AI and ML into 3D printing has opened new avenues for precision manufacturing, material design, and biomedical applications.

Biswas et al. [376] reviewed the application of AI in 3D printing of polymer microneedles (MNs), highlighting advancements in product quality control, drug release optimization, drug selection, and application development. They emphasized that integrating deep learning with reinforcement learning (RL) enables optimization of printing parameters, paving the way for fully autonomous production and evaluation of 3D-printed polymers without human intervention [377].

Beyond process optimization, AI has also enabled formulation innovation. Elbadawi et al. [378] achieved a significant milestone by successfully 3D-printing AI generated de novo formulations derived from CGAN with a fused deposition modeling (FDM) printer.

In the domain of tissue and organ engineering, Chen et al. [183] conducted a comprehensive review of AI-driven 3D bioprinting, highlighting recent advancements in AI-enabled in situ printing technologies. Similarly, Logeshwaran, Elsen and Nayak [379] explored AI-assisted structural screening and 3D design strategies for bone scaffolds, focusing on porous architectures and vascular integration relevant in both preclinical and clinical applications.

Ma et al. [15] developed a machine learning-based strategy to enhance the 3D printing fidelity of vat photopolymerization by establishing correlations between greyscale pixel combinations and cured pattern profiles. The appearances of printed samples were recorded in a database and used to train the machine learning model, with CGAN employed for data augmentation.

In summary, while AI and ML applications in 3D printing have predominantly focused on process control and engineering optimization, recent advances still demonstrate their potential in guiding material and formulation design to achieve specific printing outcomes with greater precision and functionality.

3.7 | Challenges Remaining

Although a wide variety of ML/AI models have been developed to address various polymer-related tasks, challenges persist across different scenarios, as indicated in Table 3.

4 | Critical Assessment and Comparison of Modeling Approaches

Several predictive modeling methods are available to inform 3D printing processes relating to polymers. These methods may be data-driven or rooted in the underlying physics. They may also be some combination of the two, deriving benefits from both model types. Selection of an appropriate method for a particular application is vital, and requires a broad understanding of the current research landscape, as well as validation of potential

TABLE 3 | Challenges and associated insights in leveraging ML/AI for the discovery of 3D printable polymeric materials.

Challenge	Insights	Key factors
Limited training data	The accuracy of testing results typically improves with a larger data quantity [283].	High-throughput experiments are required for high-quality datasets for 3D printable polymeric materials.
Computational cost	The cost varies from case to case. Substantial computational resources are required for sophisticated models [333].	Advanced hardware, such as GPUs, is necessary to handle and process large datasets.
Model development	Difficulty in understanding the decision-making process of the models due to their black-box nature.	Interdependent 3D printing parameters as input and hyperparameters for fine-tuning.
Data pre-processing	The generation and selection of efficient input are still challenging. As highlighted in the polymer informatics section, the effective representation of polymers is crucial for model training.	Labor-intensive tasks are required for polymeric data preparation, such as data cleaning, feature selection, label encoding, and standardization.
Data partitioning strategy	Essential for preventing overfitting, ensuring model generalization, and maintaining a fair representation of data.	Specialized splitting strategies are necessary for a fair representation of data.

methods against established data in relevant areas of chemical space. Different methods have different benefits, which tend to trade off against each other. Some problems may require a high level of chemical detail to fully explain observed phenomena, while others may seek broad and fast application to a large number of systems. The rise of AI and ML is rapidly transforming the accessibility of such large-scale studies, but as the area develops, interpretability and chemical detail must be actively maintained. Table 4 summarizes the method types discussed in this work, indicating their computational cost, chemical detail, and the types of 3D printing problems to which they may be applied.

Chemical detail can be maximized by using quantum chemistry methods, which have their basis in fundamental chemistry and include explicit modeling of electronic structure and interactions. They can be used to examine reaction mechanisms inherent to 3D printing processes, and electronic properties, which are inaccessible to several other physics-based models. However, the high computational cost of quantum chemistry significantly restricts its applicability, making complete systems difficult to access. Quantum chemistry may be combined with statistical thermodynamics methods to somewhat overcome these issues. Meanwhile, relatively cheap quantum models are always under development. Recently, Grimme announced G2-XTB a semiempirical model with DFT-level accuracy [380]. As more and faster methods continue to be developed, the role and capabilities of quantum chemistry will continue to expand. However, alternative methods are often necessary for modeling the large polymer systems relevant to 3D printing. These can include methods with a physical basis, maintaining varying levels of chemical detail. Force field methods, even those which are relatively computationally expensive such as reactive atomistic force fields, can access larger systems than quantum chemistry, and cheaper force field approaches such as coarse graining can allow property prediction on systems representative of long polymer chains. Meanwhile, ML is emerging as an option to augment existing modeling approaches such as MD, with ML interatomic potentials used to reproduce quantum energy evaluations at much lower cost. ML potentials have not yet been widely used in 3D printing studies, but they have the potential to facilitate powerful predictions.

While these physics-based models remain essential for understanding fundamental polymer behavior, data-driven methods have become increasingly valuable for extending predictions to larger chemical spaces and diverse processing scenarios. As illustrated in Section 3, QSPR models and other classical ML approaches can rapidly estimate key properties such as glass transition temperature, viscosity, or mechanical strength based on easily-computed descriptors, avoiding the need for repeated high cost simulations. More advanced deep learning frameworks can capture complex, non-linear relationships within experimental or simulated data to predict material performance under different 3D printing conditions. Such data-driven models can significantly accelerate materials discovery and process optimization, but their predictive accuracy depends strongly on the quality, quantity, and diversity of training data. In practice, combining physics-based and data-driven methods using simulation or experimental data to train and validate ML/AI models, or using ML to train interatomic potentials for use in physical modeling, can offer an effective balance between chemical detail, computational speed, and broad applicability for polymer design and additive manufacturing.

5 | Conclusion

Computational approaches are becoming increasingly vital in our development and understanding of chemistry, and these advances have the potential to benefit areas dependent on materials progress, such as additive manufacturing.

Physics-based simulations are essential for understanding the fundamental behavior of polymers in additive manufacturing.

TABLE 4 | Summary of computational methods that may be used to model 3D printable formulations and 3D printed systems, with comments on their speed, level of chemical detail, and the 3D printing problems to which they are applicable.

Method		Speed	Chemical detail	3D printing applicability
Quantum chemistry simulations		Very slow, but variation between different quantum models	Very high, includes full atomic detail and modeling of electronic structure and behavior	Reaction mechanism elucidation and kinetics, electronic property modeling. Commonly applied only to a few systems at once, and to short fragments in place of polymers.
Reactive fields	Force	Fairly slow	Atomic structural and geometric detail, electronic detail only implied by bonding	Simulations of polymerization process, can predict related properties, for example, gel point. Energetics and dynamics rely on slower variants.
Atomistic, reactive fields	Non-force	Medium speed	Atomic structural and geometrical detail, but no electronic detail	Property prediction for ink formulations and some property prediction of polymer chains; often truncated to tens to hundreds of repeat units in diluted systems.
Coarse graining		Fairly fast	Some structural detail, but on the level of groups of atoms rather than single atoms	Property prediction for large systems; must be established that models can adequately represent more detailed models before use.
QSAR/QSPR and classical ML models		Very fast once trained	Low to moderate: relies on predefined descriptors, not explicit atomic detail	Predicts bulk properties (e.g., glass transition temperature, viscosity, mechanical strength) for candidate polymers and formulations without expensive simulations, classical ML can be applied for process parameter optimization. Useful for rapid screening of large virtual libraries. The classical ML models performance can be constrained by feature selections.
Deep learning (NN, CNN, GNN)		Fast to moderate once trained; training can be computationally intensive	Can implicitly capture complex structure–property relationships but requires high-quality, curated input features	Used for predicting structure–property relationships, generative design of novel polymer structures, and mapping processing–property links. Needs large, diverse datasets for reliable generalization.
Hybrid ML–physics models		Moderate	Combines moderate chemical detail from physics-based simulations with data-driven corrections	Balances computational efficiency and accuracy by incorporating physics based constraints into ML predictions. Useful for inverse design, property tuning, and uncertainty quantification for 3D printable polymers.

Techniques such as molecular dynamics and quantum chemistry provide detailed insights into polymer conformations, electronic properties, and reaction mechanisms, and these methods have been successfully applied to predict critical parameters such as viscosity, solubility, and gel point, which influence both the printability and performance of 3D-printed parts. While computationally intensive, these approaches offer high accuracy and mechanistic interpretability, making them indispensable for modeling complex polymer systems. As computational power and efficient algorithms continue to evolve, significant opportunities lie in modeling the complex mechanisms that give rise to the robust and resilient materials desired in additive manufacturing, as well as those in more application specific areas, such as bioprinting.

Machine learning and artificial intelligence, whilst long standing activities, have recently emerged as powerful tools for accelerating polymer discovery. By learning structure–property relationships from experimental and simulated data, these models enable rapid screening of candidate materials and prediction of key properties such as glass transition temperature, mechanical strength, and degradation behavior, all of which are necessary for materials selection. The integration of simulation data into ML workflows enhances model performance and expands the accessible design space. Despite challenges related to data quality and representation, data-driven approaches are increasingly central to the development of functional and sustainable 3D-printable polymers.

Effective polymer informatics is critical for enabling predictive modeling. Advances in molecular representations, including SMILES, BigSMILES, and graph-based encodings, have improved the ability of ML models to capture the structural complexity of polymers. Descriptor-based and fingerprinting methods continue to play a key role in property prediction, while hierarchical and graph neural network approaches offer promising avenues for future development. Accurate and scalable representations are essential for training robust models and ensuring generalizability across diverse polymer classes. However, challenges remain in the representation of large, temporally evolving molecules, and how to handle simulation problems that quickly span multiple length scales.

Generative models, including variational autoencoders, generative adversarial networks, and large language models, are transforming the landscape of polymer design. These tools enable inverse design by generating novel polymer structures with targeted properties, guided by learned distributions from existing data. Applications range from the design of printable formulations to the optimization of mechanical and thermal properties. As these models mature, they are expected to play a central role in the autonomous discovery of next-generation materials. An existing weakness of all these types of models is the accessibility of sufficiently large and sufficiently reliable data to enable precision in the predictions. In the future, the interoperability of databases and careful integration of workflows and data collection protocols with databases will begin to alleviate some of these bottlenecks and allow robust, reliable and transparent predictions.

The continued advancement of predictive approaches in 3D printing will depend on the availability of large, high-quality datasets with standardized formats and comprehensive metadata, supported by collaborative efforts to develop open-access databases and improve data interoperability. Integration of physics-based and data-driven methods offers a promising path forward, reducing computational time whilst also increasing precision. As computational resources and algorithmic capabilities expand, predictive modeling will become an increasingly vital component in the design of high-performance, sustainable polymeric materials for additive manufacturing. We will see their impact on all stages of 3D printing; in the selection, design and synthesis of materials, on their processing and polymerization during production and in predicting their properties and how they evolve during use. These methods have the potential to streamline, improve and innovate materials design in many areas, and it is clear that disruptive, emerging technologies such as 3D printing are ripe for their deployment.

Author Contributions

Isabel Cooley: conceptualization (equal), writing – original draft (equal), writing – review and editing (equal). **Weiling Wang:** conceptualization (equal), writing – original draft (equal), writing – review and editing (equal). **Vladimir Kozyrev:** conceptualization (supporting), writing – original draft (supporting), writing – review and editing (equal). **Ricky D. Wildman:** funding acquisition (equal), resources (equal), writing – review and editing (equal). **Blair F. Johnston:** funding acquisition (equal), resources (equal), writing – review and editing (equal). **Anna K. Croft:** conceptualization (lead), funding acquisition (lead), project administration (lead), resources (equal), writing – original draft (supporting), writing – review and editing (equal).

Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

Data sharing does not apply to this article as no new data were created or analyzed in this study.

Related WIREs Articles

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