The Solution is the Solution: Data-Driven Elucidation of Solution-to-Device Feature Transfer for π-Conjugated Polymer Semiconductors

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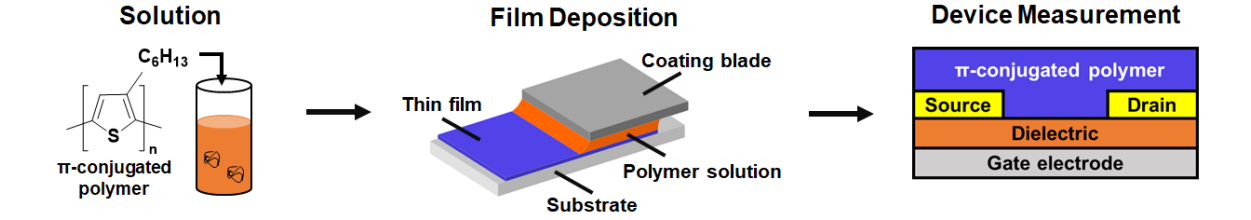
Abstract

The advent of data analytics techniques and materials informatics provides opportunities to accelerate the discovery and development of organic semiconductors for electronic devices. However, developing engineering solutions is limited by the ability to control thin-film morphology in an immense parameter space. The combination of high throughput experimentation (HTE) laboratory techniques and data analytics offers tremendous avenues to traverse the expansive domains of tunable variables offered by organic semiconductor thin films. This Perspective outlines steps required to incorporate a comprehensive informatics methodology into experimental development of polymer-based organic semiconductor technologies. The translation of solution processing and property metrics to thin-film behavior is crucial to inform efficient HTE for data collection and application of data-centric tools to construct new process–structure–property relationships. We argue that detailed investigation of the solution state prior to deposition in conjunction with thin-film characterization will yield deeper understanding of the physicochemical mechanisms influencing performance in π-conjugated polymer electronics, with data-driven approaches offering predictive capabilities previously unattainable via traditional experimental means.

1. Introduction

The last decade has seen significant interest in the development of new π-conjugated polymer chemistries for the fabrication of lightweight, printable, low-cost, deformable, and large-area devices,[1-2] including organic photovoltaics (OPV),[3-4] organic field-effect transistors (OFET),[5-6] and organic light-emitting diodes (OLED).[7] However, the chemistry and processing of polymer candidates form a complex design space that is inefficient to explore via trial and error.[8] After almost 30 years of research, homopolymers like poly(3-hexylthiophene) (P3HT) have largely plateaued in performance, with maximum charge-carrier mobilities on the order of 1 $cm^2V^{-1}s^{-1}$ in devices.[9] More recently, families of donor–acceptor (D-A) (or "push-pull") copolymers have been developed that rival or even surpass (>10 $cm^2V^{-1}s^{-1}$) the performance benchmark of amorphous silicon in thin-film transistors (0.5-1 $cm^2V^{-1}s^{-1}$).[10-11] Efficiently traversing the D-A design space requires thoroughly understanding the sensitivity of device performance to polymer chemistry, morphology, and other key process–structure connections – a foundation of understanding yet to be fully attained.

Design developments in organic semiconductors have traditionally arisen through Edisonian experiments or simulations. For a single polymer candidate, the space of solution process parameters encompasses a wide range of tunable variables,[12-16] as shown in Figure 1. Candidate material discovery is often a separate research endeavor from process optimization, although they are related by the grand objective of controlling structural features within the immense design space offered by the independent variables of interest.



Polymer	Solution	Deposition	Substrate	Device Performance

• Monomer chemistry
• Molecular weight
• Polydispersity
• N-type/P-type/ ambipolar
	• Concentration
	• Blend composition
	• Solvent:
	  • Volume fraction
	  • Boiling point
	  • Hansen radius
	• Aging time and temperature
	• UV irradiation
	• Sonication
	• Environment
		• Spin coating:
		  • RPM
		  • Time
		• Blade coating:
		  • Coat speed
		  • Blade angle
		  • Direction
		• Temperature
		• Film thickness
		• Annealing
			• Surface treatment
			• Electrode configuration
			• Electrode material
			• Channel dimensions
			• Dielectric material
			• Dielectric thickness
				• Mobility
				• Threshold voltage
				• On/off current ratio
				• Environment (air, N_2, etc.)
				• Transfer curve regime

Figure 1. Diagram depicting the variety of fabrication and characterization parameters for π-conjugated polymer-based organic field-effect transistor and associated processing variables. Adapted with permission from ref. 16. Copyright 2016, Elsevier.

Because traditional approaches to enhance the performance of organic semiconductors often incur high time and resource costs, recent computer-aided approaches have accelerated organic semiconductor research with promising early results. Computational modeling methods accelerate both the process of high-throughput candidate discovery and the investigation of structure–property relationships.[17-24] To bridge the experimental data gap, high-throughput experimental methods integrate customized hardware with machine learning to optimize workflows with combinatorial deposition techniques,[25-27] high-throughput characterization suites,[26-29] and self-driven laboratories.[30-32] However, many approaches focus on thin-film characterization without characterizing the solution phase as well; neglecting solution-state behavior and the effects of key process parameters introduces significant variance to the final measured thin-film properties.

The collection and curation of large databases representative of the target phenomena is a bottleneck in the development of comprehensive informatics methodologies. While studies have produced sizable databases of screened candidate materials with properties simulated through a variety of computational approaches,[17-18, 33-35] these databases do not screen for solution-state behavior and often do not incorporate the principles of findable, accessible, interoperable, and reusable (FAIR) data.[36] The modern emphasis on data-driven methods underscores the need for collaborative and open-source databases of building block, material, and device characteristics for organic semiconductors. Crucially, these databases must incorporate the full thin-film processing history. Once such databases have been populated and curated, intelligent cheminformatics methods are necessary to extract meaningful data.

In this Perspective, we emphasize the importance of interrogating solution-state behavior to better understand the role that the solution-to-film process plays in regulating device performance. First, we discuss key solution-state and thin-film characteristics to which organic semiconductor performance is known to be sensitive, highlighting recent efforts to rationalize connections between the solution and thin-film states. We then provide an overview of early computer-aided methodologies for developing high-performance organic semiconductors while identifying opportunities for further interrogation of solution state behavior. Finally, we present an outlook for integrated experimental and computational workflows that capture the information necessary to efficiently explore the solution-to-film design space for π-conjugated polymers for organic semiconductors.

2. Rationalizing Solution-to-Film Processing in Organic Semiconductors

2.1. Deposition

Polymer semiconductors are typically deposited as thin films from solution-based inks.[37] Literature highlights the roles of the solution processing history and deposition parameters in regulating polymer self-assembly and crystallization.[38-39] Compared with traditional spin coating methods, meniscus-guided coating (MGC) techniques (such as blade coating or solution shearing)

require a smaller amount of solution and better represent large-scale production processes.[13, 40-41] Previous studies of π-conjugated polymer films deposited via MGC identified shear speed, solution concentration, solvent choice (i.e., solvent boiling point, polymer–solvent interactions, etc.), and deposition temperature as four elementary deposition factors that regulate precise control of the thin-film morphology and electronic performance.[12-13, 38, 42]

In MGC techniques, competition between capillary forces induced by solvent evaporation and viscous forces imposed by the blade or substrate results in three deposition regimes as a function of the shear speed.[12-13, 38, 40] Deposition at shear speeds between the lower (evaporative) and higher (Landau–Levich) shear speed regimes can help to planarize the polymer chain backbone even for D-A copolymers, improving intrachain charge-carrier transport.[38] The shear speed boundaries between these regimes vary depending on the choice of semiconducting polymer and solvent, as well as on the solution viscosity. The thin-film crystal growth rate is also strongly influenced by the deposition temperature, solution concentration, and solvent quality,[12, 43] enabling further tuning of the charge-carrier mobility.[44]

2.2. Solution-State Processing and Characterization

Optimizing the performance of organic semiconductor devices requires elucidating the complex relationships between solution-state aggregation, solid-state morphology, and charge-carrier transport. Recent work has revealed that aggregates formed in solution before deposition directly influence solid-state structural features in deposited films,[45-46] as depicted in Figure 2. The enhanced backbone planarization within D-A polymer chains enables strong intramolecular charge transfer,[47] which might contribute to aggregation observed even in extremely dilute solutions. Therefore, rationalizing aggregation in solution offers a direct pathway to control thin-film morphology.[48]

The amount of solution-state aggregation can be tuned via parameters such as the relative polymer–solvent interactions (solvent quality),[45,49] solution concentration,[50] dissolution temperatures,[46] aging time,[51] UV-induced nucleation,[52] and ternary-component blending.[53] Poor solvent conditions enhance solution-state aggregation, with lower deposition temperatures helping to preserve the developed aggregates. By contrast, solution-state polymer aggregation is suppressed in good solvent conditions, requiring higher deposition temperatures to provide enough thermal energy for rapid aggregation and thin-film crystal growth.[43]

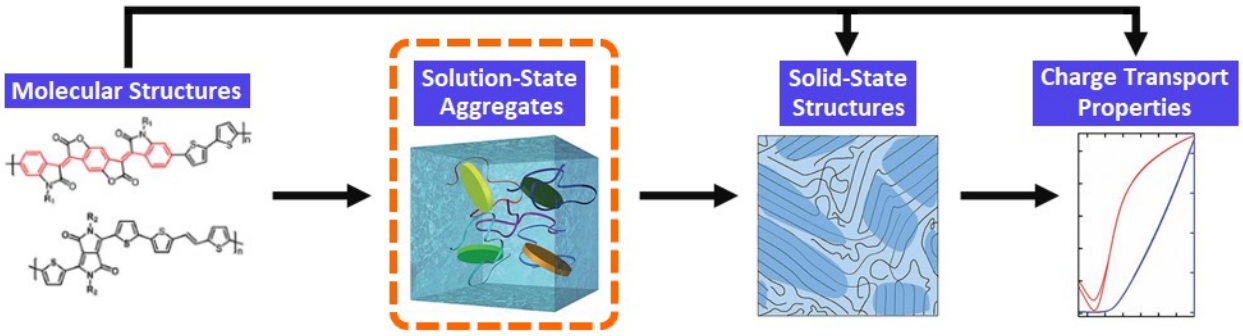


Figure 2. A representative pipeline for understanding the structure–property relationship in polymer semiconductors. Reprinted and adapted with permission from ref. 45. Copyright 2017, John Wiley and Sons.

Unfortunately, a generalized understanding of polymer self-assembly and solution-state aggregation remains elusive. The relatively high absorption coefficients in the visible and near-IR regions prohibit common micro- and spectroscopic techniques from directly probing the polymer solution state. The strong absorption within these regions is enhanced in D-A polymers, due to a more rigid backbone and longer persistence length. This issue can be circumvented by significantly reducing the optical path length in order to clarify continuous variations in aggregate–amorphous region transformation through *in-situ* temperature-dependent absorption spectroscopy.[54-55] Alternatively, freeze-drying samples allows the solution-state conformations to be captured and preserved into the solid state, paving the way for common solid-state characterization techniques.[45, 56]

Scattering techniques such as dynamic and static light scattering (DLS and SLS) and small angle X-ray and neutron scattering (SAXS and SANS) have been employed for direct interrogation of chain conformations and polymer aggregation in solution. DLS and SLS can provide quantitative estimates of the hydrodynamic radius and radius of gyration of dilute solutions,[46] respectively, while the strong penetrating ability of SANS measurements offers high resolution of structural features across a wide concentration range.[57] For example, Zheng et al. demonstrated that D-A polymers form one-dimensional rod-like structures in good solvent conditions, while forming two-dimensional lamellar structures in poor solvent conditions.[45]

3. Integrated Experimental–Computational Approaches

3.1. Computational Modeling

Efficient charge-carrier transport in π-conjugated polymer devices is influenced by a wide range of factors from the electronic scale to the device scale, but accessing larger length scales through computational modeling approaches generally requires sacrificing the resolution of phenomena occurring at smaller scales. Thus, multi-scale simulation design leveraging the

strengths of each technique to resolve phenomena at the relevant length scale is essential to modeling D-A polymers.[58] Quantum chemical methods can resolve optoelectronic properties (e.g., band gap, absorption spectra, etc.), while molecular dynamics (MD) approaches enable direct simulation of chain dynamics in solution and in melt. Further insights into the effects of solution-phase morphological assembly can be obtained through stochastic MD algorithms (e.g., kinetic Monte Carlo) or through coarse-graining procedures (e.g., iterative Boltzmann inversion).

MD studies suggest that solution-phase aggregation has far-reaching consequences on thin-film morphology and performance,[59-60] but the full implications of solution-phase aggregation on the resultant device performance have not been thoroughly explored. Fortunately, the literature provides promising avenues for in silico interrogation of solution-to-film feature transfer. Simulation studies have modeled the aggregation of π-conjugated polymer chains in solution and in melt,[61-63] the nucleation and growth of thin films on explicitly modeled substrates,[21, 64-65] and atomistic models of solvent evaporation.[66-68] Combining these approaches forms a robust computational pipeline for investigating the ramifications of solution-phase aggregation, as demonstrated in recent atomistic MD studies that model microsecond-scale evaporation processes to reveal salient features of π-conjugated thin-film growth on substrates.[66-67]

3.2. High-Throughput Experimentation

High-throughput experimentation (HTE) methods present a promising path to screen the complex solution and deposition spaces offered by π-conjugated polymers. The automated deposition of π-conjugated polymers into libraries – combinatorial samples that vary composition, thickness, or other parameters – has been carried out in both discrete and gradient formats.[23] The applicability of MGC approaches to continuous printing processes makes them especially relevant to gradient films. For example, gradient thin-film libraries of composition, thickness, or other process parameters can be produced by blade coating. Such approaches allow full consideration of deposition parameters, but require further correlation between small sample-scale and practical device-scale fabrication.

Efficient library characterization exploits HTE to rapidly probe the deposited thin-film microstructure. Spectroscopic and beam-based methods are especially conducive to high-throughput characterization, as point-by-point measurements can be spatially processed to generate large volumes of data. For example, Harillo-Baños et al. used a suite of hyperspectral imaging techniques to extract spectroscopic information from library samples generated by sequential coatings.[27] UV–Vis, Raman, photoluminescence, and X-ray spectroscopy, which are useful for interrogating π-conjugated polymer structures, have already shown success in characterizing libraries in HTE workflows.[23, 69]

Additionally, a necessary inclusion in characterization suites is the collection of key device metrics (e.g., charge-carrier mobility or power conversion efficiency) such that structural

characteristics can be mapped to device performance.[8] Automatic techniques have been developed to probe electrical characteristics of thin films. For example, rapid combinatorial screening for both OPV and OFET device characterization has been demonstrated using array-based designs.[25, 70] However, device measurements can be challenging to compare across datasets due to inherent variation due to different measurement settings and curve fitting semantics (e.g., measurement environment, current ranges, saturation vs. linear regimes, etc.).[10, 71] When reporting information on device performance, these settings and metadata should also be reported.[72]

3.3. Machine Learning Integration for Experimental Workflows

Machine learning (ML) techniques can accelerate materials discovery by identifying patterns that are difficult to reveal via scientific intuition alone,[33] as long as sufficient amounts of representative data are available. The capability of HTE to generate large volumes of data in a short time necessitates the use of ML techniques to expedite the exploration of multivariate design spaces and provide advanced data analysis, as the effectiveness of HTE is diminished if successive experiments are unguided. ML allows data generation to be informed intelligently in a comprehensive workflow of experimental design and sequential learning.[73]

More recently, the emergence of the self-driven laboratory concept has given rise to automated, intelligent experimental workflows that accelerate experimental data generation by orders of magnitude, with progress in developing materials for OPVs.[30-31] For example, Du et al. screened the thin-film device efficiency and photostability of over 100 combinations of composition and deposition parameters using an autonomous platform, with successive experiments informed by an embedded Gaussian process model.[32] These workflows establish an important foundation for automated development of π-conjugated polymer semiconductors, but these methodologies could benefit from considering additional factors, such as solution-state measurements and MGC-based deposition methods.

4. Perspective and Outlook

The importance of developing and deploying π-conjugated polymers as advanced, modern organic semiconductors motivates fundamental studies toward further control over polymer thin-film morphology. A combination of "low-throughput" studies by domain experts has accumulated a growing body of evidence that solution-state and thin-film deposition parameters are crucial to optimizing D-A polymer device metrics. In parallel, the progress made in the organic semiconductor space has mobilized domain-equipped data scientists and engineers to design data-driven, HTE methodologies dedicated to investigating these materials. A tremendous challenge in applying autonomous or high-throughput discovery methods is obtaining relevant process–structure information that captures the sensitivity of device performance to relevant properties.

Enabling characterization of the polymer structure in solution should guide high-throughput workflows toward unearthing new superior candidates or design rules. Spectroscopic

techniques (absorption and photoluminescence) have already been leveraged for thin-film characterization. More comprehensively capturing the complex propagation of aggregate structures to the resultant solid-state film requires extending these spectroscopic techniques to solution characterization. Development of high-throughput characterization suites should also consider the modularity of these solution measurement components, to accommodate evolving research directions. Successful implementation would in turn enrich datasets for computational modeling and cheminformatics methodologies.

High-throughput solution-state characterization has already been demonstrated for other applications. Epps et al. recently reported on autonomous discovery of perovskite quantum dots using a customized flow system, enabling in situ characterization of photoluminescence and UV–Vis absorption using reduced path lengths.[74] High-throughput SAXS measurements have also been performed on microliter volumes of protein structures with automated sample handling.[75-76] Although there are technical and infrastructural roadblocks to enabling certain characterization techniques as self-contained workflows, e.g., high-energy or synchrotron-based measurements, the increasing availability of high throughput SANS with automated structural analysis at national laboratories facilitates acquisition of larger datasets of solution-state structural parameters.[77-82]

Additionally, accurate scaling between combinatorial libraries and larger-scale samples must be established. Experimental workflows should employ MGC deposition modules and other industrially relevant processing components to facilitate correlation of small-scale experiments to the deployment level, as polymer–solvent interactions specific to the processing method affect the transition to the thin film. While thickness, composition, and temperature have been explored, for example, accurately capturing the effects of structures that develop in solution due to specific processing conditions like solvent tuning or aging in an HTE format could offer further control of thin-film microstructure and device performance. Other process-specific phenomena, such as solution inhomogeneity or edge effects, may interfere with structural development in both solution state and thin film. The potential interference of such effects should be explored and mitigated in future HTE studies.

In this Perspective, we presented a series of key factors to consider in rationalizing the influence of solution-state and thin-film factors on device metrics obtained when π-conjugated polymers are used as the active material. The directions and approaches proposed herein aim to engender further collaboration among experimental and computational domain experts and domain-equipped data scientists to tackle the complex, multivariate challenges in developing the next iteration of polymer semiconductors. By combining new tools under development in each domain with longstanding domain expertise, we envision a rapid increase in the ability to co-design polymers and processing modalities that offer semiconductors with finely tuned electronic, redox, optical, and mechanical characteristics.

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TOC Graphic: