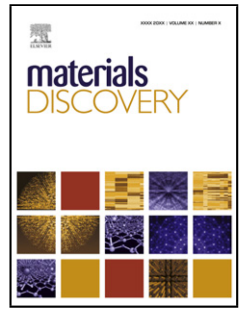
Accepted Manuscript



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PII: S2352-9245(17)30048-0
DOI: https://doi.org/doi:10.1016/j.md.2018.06.002
Reference: MD 49

To appear in:

Received date: 18-12-2017
Revised date: 9-6-2018
Accepted date: 17-6-2018

Please cite this article as: Spencer Pfeifer, Balaji Sesha Sarath Pokuri, Pengfei Du, Baskar Ganapathysubramanian, Process optimization for microstructure-dependent properties in thin film organic electronics, *<![CDATA[Materials Discovery]]>* (2018), https://doi.org/10.1016/j.md.2018.06.002

Process optimization for microstructure-dependent properties in thin film organic electronics

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Abstract

The processing conditions during solvent-based fabrication of thin film organic electronics significantly determine the ensuing microstructure. The microstructure, in turn, is one of the key determinants of device performance. In recent years, one of the foci in organic electronics has been to identify processing conditions for enhanced performance. This has traditionally involved either trial-and-error exploration, or a parametric sweep of a large space of processing conditions, both of which are time and resource intensive. This is especially the case when the process → structure and structure → property simulators are computationally expensive to evaluate.

In this work, we integrate an adaptive-sampling based, gradient-free, Bayesian optimization routine with a phase-field morphology evolution framework that models solvent-based fabrication of thin film polymer blends (process → structure simulator) and a graph-based morphology characterization framework that evaluates the photovoltaic performance of a given morphology (structure → property simulator). The Bayesian optimization routine adaptively adjusts the processing parameters to rapidly identify optimal processing configurations, thus reducing the computational effort in *process* → *structure* → *property* explorations. This serves as a modular, parallel 'wrapper' framework that facilitates swapping-in other process simulators and device simulators for general process → structure → property optimization. We showcase this framework by identifying two processing parameters, the solvent evaporation rate and the substrate patterning wavelength, in a model system that results in a device with enhanced photovoltaic performance evaluated as the short-circuit current of the device. The methodology presented here provides a modular, scalable and extensible approach towards the rational design of tailored microstructures with enhanced functionalities.

Keywords: Bayesian Optimization, Process–Structure–Property, Substrate Patterning, Morphology, Process design

1. Introduction

The field of organic electronics continues to grow at a rapid pace, delivering a number of emerging technologies with disruptive potential [1–5]. This includes organic photovoltaics (OPVs) [5, 6], light-emitting diodes (OLEDs) [4, 7], transistors (OFETs) [8, 9], memory diodes [10, 11], and energy storage devices [12], to name a few. This broad appeal stems from a set of unique properties inherent to these devices; namely, the full range of electronic functionalities packed into an ultra-thin yet flexible form factor [4]. Moreover, such devices may be sustainably produced at low-costs through established high-throughput printing processes [13, 14]. With the increasing availability of biodegradable and nontoxic organic materials, these scalable printing techniques are expected to pave the way for disposable designs with minimal environmental impact - marking a significant step towards a fully-sustainable product development pipeline [15].

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