AI/ML/Autonomous Experimentation for Thin Films Processing

Room 317 - Session AIML1-FrM

Materials Design and Autonomous Discovery

Moderators: Eden Goodwin, Carleton University, Canada, **Prof. Stephanie Law**, Pennsylvania State University

8:15am **AIML1-FrM-1 Accelerating Discovery and Design for Thin Film Polymer Self-Assembly through Machine Learning**, ***Gregory Doerk,*** Brookhaven National Laboratory **INVITED**

Thin film polymer self-assembly is a powerful approach to create nanoscale patterns across large areas with low cost for diverse applications in electronics and materials science. The confluence of compositional and architectural variation, entropic and surface energy constraints arising from thin film confinement, and process-dependent assembly pathways yields of panoply of nanoscale morphologies of which only a fraction can be discovered, catalogued, and engineered through manual experimentation. This talk will elaborate examples where artificial intelligence and machine learning (AI/ML) can accelerate thin film polymer self-assembly research. We describe the application of Gaussian process regression to automate x-ray scattering characterization for the discovery of new morphologies in template-directed self-assembly of block copolymer blends. We then illustrate the application of an active learning approach that incorporates foundation model-supported “few shot” image classification for determining processing-morphology relationships in spray-deposited block copolymer/homopolymer blend films using minimal quantities of data. Complementary in situ x-ray scattering measurements during spraying provide key mechanistic insights into trends in self-assembled structural organization across the process design space.

8:45am **AIML1-FrM-3 Autonomous Discovery of PFAS-Free Low Surface Energy Thin Films**, ***Stanley Lo,*** *Abraham Herzog-Arbeitman, Alan Aspuru-Guzik, Helen Tran, Nipun Gupta, Harrison Mills,* University of Toronto, Canada

Per- and polyfluoroalkyl substances (PFAS) have long dominated low-surface-energy coatings due to their exceptional water and oil repellency. However, regulatory pressure and environmental persistence concerns have created urgent demand for fluorine-free alternatives. Rational design of such materials requires systematic exploration of polymer composition–wettability relationships, a challenge ideally suited to autonomous experimentation.

We present a self-driving laboratory for accelerated discovery of PFAS-free polymer thin films with low surface energy. The platform integrates a continuous-flow reactor, an automated fraction collector for composition-resolved sample handling, a spin coater for reproducible thin-film deposition, and a multi-liquid dynamic contact angle goniometer for comprehensive wettability characterization. Closed-loop control enables autonomous navigation of copolymer composition space.

The chemical system employs ring-opening metathesis polymerization (ROMP) of norbornene-based monomers to produce statistical polynorbornene copolymers. Monomer design is grounded in the Hansen solubility parameter (HSP) framework, which decomposes intermolecular interactions into three orthogonal dimensions: dispersion (δD), polarity (δP), and hydrogen bonding (δH). Three monomers were synthesized with side groups systematically representing each dimension: an apolar aliphatic chain (low δP, low δH), a polar non-protic group (high δP), and a polar hydrogen-bonding group (high δH). ROMP copolymerization of these monomers yields materials with continuously tunable surface chemistry across the HSP space.

Dynamic contact angle measurements using multiple probe liquids (water, ethylene glycol, and hexadecane) enable surface free energy decomposition and discrimination between hydrophobic and oleophobic character. The platform iteratively selects compositions, deposits films, measures wettability, and updates a surrogate model to identify low-surface-energy optima without fluorinated components.

This work establishes a generalizable, data-driven framework for discovering sustainable high-performance surface coatings and provides mechanistic insight into how monomer polarity and hydrogen-bonding capacity govern macroscopic wettability.

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