

## Coupled Machine Learning and High Throughput Development of Polymer Blends

Carson Meredith, School of Chemical & Biomolecular Engineering

Elsa Reichmanis, School of Chemical & Biomolecular Engineering

Martha Grover, School of Chemical & Biomolecular Engineering

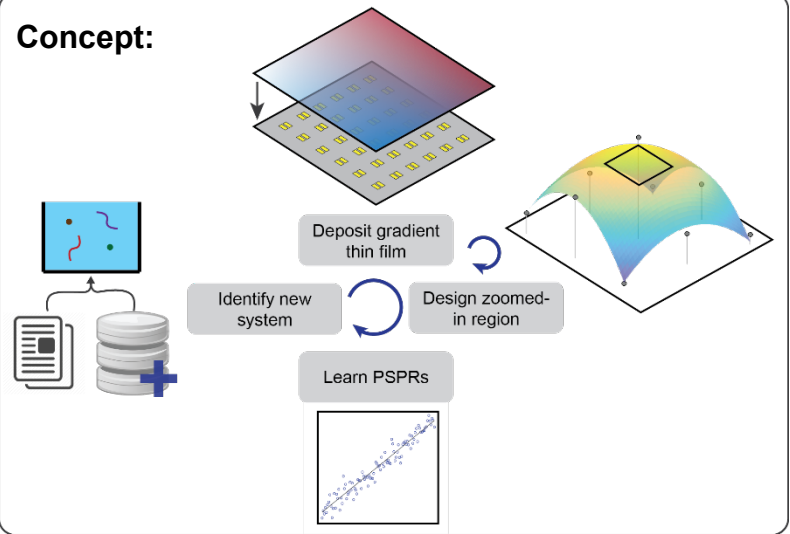
**Objectives:** Combine machine learning for experimental design with experimental composition, temperature and thickness libraries to discover polymer blends with enhanced mechanical and thermal properties. Carry out multifunctional property optimization for industrially-relevant applications.

### Technical Approach:

**Computational:** Build models from experimental data, utilizing empirical and machine learning approaches, and integrating physically based mathematical models when available. Employ sequential experimental design to design each new gradient library.

**Experimental:** Initially, libraries of polymer blends can be fabricated through physical mixing of polymer solutions in common solvents. Solution-based deposition of films with controlled composition and temperature (deposition or annealing) will allow exploration of parameter space with existing methods in the Meredith lab. Eventually a melt-based approach to polymer blending should be developed, but the solvent-based is a first-order screen of composition and temperature effects. Property screening will focus on mechanical properties (with HTMECH) and their dependence on thermal and solvent exposure (heat and oil resistance).

### Concept:



**Impact:** Multicomponent, multiphase mixtures of polymers are used in many if not most engineering applications of plastics. These have included traditional thermoplastics and thermosets, but also show promise for eventual use in 3D printing. However, the complex interaction between phase behavior, mechanical properties, thermal history and composition is still a challenge to product development. A coupled approach will enable combination of the new tools emerging in machine learning with the high data volumes possible in library preparation and screening.