Materials Informatics & Machine Learning

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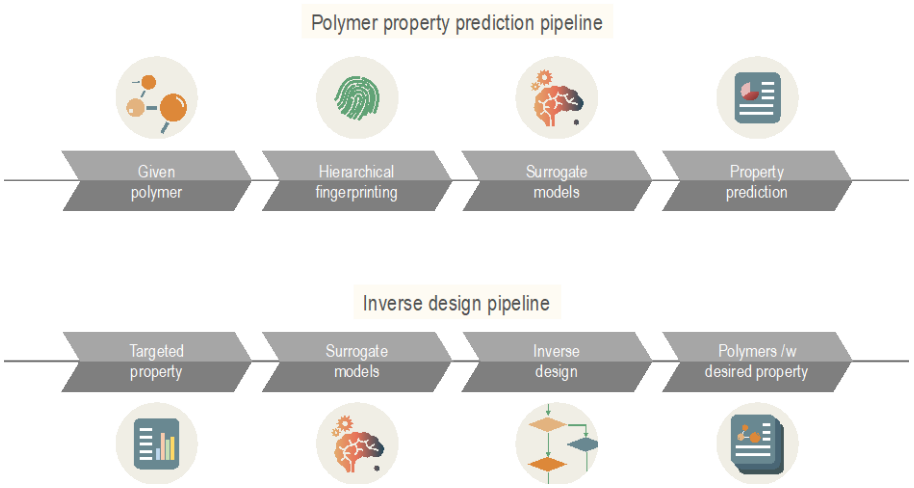
Objectives: Utilize materials data from high-throughput computations, high-throughput experiments and literature to build surrogate machine learning models to enable ultrafast, on-demand materials property predictions. Utilize this capability to help accelerate the design of materials that meet a target property and/or performance requirement.

Technical Approach: The following strategy will be pursued:

- Develop & utilize techniques to efficiently create and capture relevant materials data across chemical spaces from various sources.
- Numerically represent materials using a variety of fingerprinting and featurization techniques, as relevant for the problem.
- Develop & utilize machine learning techniques to map the fingerprint to properties, thus resulting in an ultrafast property prediction model.
- Achieve materials design using active learning and genetic methods to identify materials meeting a target performance or property metric, or the next experiment to perform.

Concept Illustration: (see also www.polymergenome.org)



Impact: Traditional materials development in industry proceeds by (1) trial-and-error, (2) intuition and (3) past experience, consuming enormous effort, time and resources. We are developing a data-driven platform to reduce cost and significantly accelerate materials discovery and development for several applications. We have applied these methods within the polymer domain, which has led to a Polymer Informatics platform called Polymer Genome (www.polymergenome.org).