Combining Physics and Machine Learning for the Modeling and Design of Complex Soft Materials

Research Statement – Shengli Jiang

My group will work at the interface of computational materials science and data science. *We will develop physics-informed computational approaches that integrate molecular simulation with machine learning to enable the rational design of soft materials* (Figure 1). Soft materials exhibit rich and tunable design properties that are governed by topological, compositional, and chemical complexity; these properties make them useful in applications such as hydrogel matrices for drug delivery [1] and polymeric membranes for water purification [2]. However, efficiently identifying optimal materials within their vast combinatorial design space remains a grand challenge [3]. While data-driven models offer potential for materials design, they often have limited physical interpretability and generalization [4]. Moreover, available databases and models used in materials design procedures are often heterogeneous, complicating their efficient use. *These technical challenges require new computational pipelines that couple molecular simulation with physics-based data representations and machine learning to uncover interpretable structure–property relationships and accelerate the design of soft materials.*

My group will focus on the physics-informed design of soft materials for energy and sustainability applications. *Instead of relying solely on data-driven methods, our approach aims to ground such methodologies in physics.* We will develop hierarchical data representations for materials that encode symmetry, topology, and chemical composition, while respecting physical constraints across molecular and mesoscopic scales. We will also construct interpretable surrogate machine learning models that are consistent with conservation laws, incorporating uncertainty quantification to overcome data scarcity and to inform experimental design. In addition, we will implement design algorithms that account for materials synthesis and processing constraints, thus narrowing down the search space and ensuring that identified candidates are experimentally viable.

Throughout my research career, I have been exposed to a broad range of interdisciplinary and collaborative experiences that uniquely position me to lead a research program that addresses these challenges. During my training, I developed expertise in the modeling, property prediction, and inverse design of soft materials using *multiscale simulation, kinetic modeling, machine learning, and uncertainty quantification* [5,6]. Collaborations with diverse experimental groups have allowed me to use my skill set to tackle challenges in applications such as sensor design [7–9], sustainability [10], solvent systems [11,12], and electrochemistry [13]. Collaborations with Department of Energy labs (Argonne and Oak Ridge) and industry (Dow, ExxonMobil, Arkema) have also allowed me to tackle impactful problems and identify new research directions.

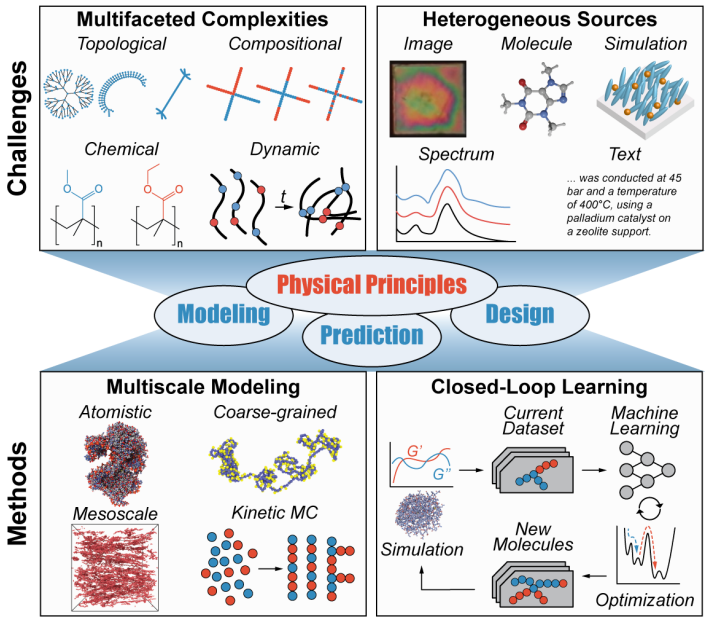

Figure 1: Overview of research interests in the Jiang Group, addressing the multifaceted challenges of soft material design (*top*) through multiscale modeling and physics-informed closed-loop approaches (*bottom*) for the modeling and design of soft materials in energy and sustainability applications.

Potential Sources of Funding: The proposed research, with applications in energy and sustainability, is fundable via numerous sources, including NSF (DMREF, CBET, Division of Materials Research, Division of Chemistry, and the National AI Research Institutes), ACS (Petroleum Research Fund), DOE (Advanced Materials & Manufacturing Technologies Office and Advanced Scientific Computing Research Program), NIH (National Institute of General Medical Sciences), as well as private foundations and industrial partners.

In the following, I outline my past and current research alongside my future plans. The three main thrusts of my future work form a *cohesive program* that bridges multiscale modeling and autonomous design of complex soft materials, *embedding physics-based representations and constraints to overcome the limitations of purely data-driven methods*. My interdisciplinary and collaborative experience, along with diverse theoretical and computational skills, *distinctly equip me to lead this vision* by tackling high-impact problems, fostering cross-disciplinary teams, and translating insights into innovations for energy and sustainability.

Past and Current Research

1. Machine Learning and Uncertainty Quantification for Materials

Design of Chemoresponsive Liquid Crystals. During my Ph.D. at the University of Wisconsin–Madison, I collaborated with Prof. Nicholas Abbott (Cornell) and Profs. Reid Van Lehn, Manos Mavrikakis, and James Schauer (UW–Madison) to develop machine learning frameworks that integrate convolutional neural networks and topological data analysis for designing chemoresponsive liquid crystals to detect trace-level gaseous analytes[7,9]. These frameworks improved detection sensitivity and interpretability while reducing computational costs through topological representations. *This work forms the basis for Thrust 1, advancing topological approaches to design complex soft materials.*

Uncertainty Quantification in Molecular Property Prediction. To enable reliable molecular modeling and property prediction, I created general methods for assessing uncertainties in predictive models, collaborating with Dr. Prasanna Balaprakash (Oak Ridge National Laboratory)[14]. These methods separate uncertainties arising from random noise in data (e.g., measurement variability) and those from lack of knowledge in models (e.g., limited training data), improving prediction accuracy across diverse chemical datasets. This approach provides actionable insights for targeted data collection and supports informed decision-making in fields like drug discovery and materials science. *This work motivates Thrust 3, which focuses on uncertainty-guided autonomous data generation for scalable materials discovery.*

2. Polymer Modeling, Property Prediction, and Inverse Design

Physics-Informed Machine Learning for Polymer Property Prediction. A key challenge in polymer science lies in creating predictive models that are both accurate and transferable across diverse polymer chemistries and architectures. I developed approaches that integrated polymer physics with graph-based machine learning techniques to improve generalizability in predicting conformational properties and phase behavior[6,15]. By embedding physical principles into data-driven methods, this framework exhibited robustness when extrapolating to out-of-distribution molecular weights, compositions, and chemical functionalities. *This work inspires Thrust 1, which emphasizes physics-informed data representations for soft materials design.*

Closed-Loop Machine Learning for Polymer Design. The vast design space of polymer topologies challenges targeted property optimization. In collaboration with Prof. Adji Bousso Dieng (Princeton), I developed a graph-based variational autoencoder that encodes diverse architectures into a continuous latent space from molecular dynamics data[5]. Integrated with Gaussian process surrogates and multiparticle collision dynamics, this enables Bayesian optimization to identify polymers matching prescribed viscosity profiles by adjusting topology and solvophobicity. By embedding physical principles, these methods uncover design degeneracies and guide extrapolation via scaling theories for extreme targets. *This work motivates Thrust 2, which focuses on physics-informed closed-loop learning.*

Molecular Simulation and Kinetic Modeling of Commodity Polymers. Commodity polymers, such as fluoropolymers, are vital materials whose properties depend heavily on molecular weight distribution and microarchitectural variations. In collaboration with industrial partners, I developed molecular dynamics and kinetic modeling frameworks to explore how branching motifs and polydispersity shape conformational, mechanical, and processing-structure-property relationships. These models established predictive design principles connecting microarchitecture to performance for next-generation commodity polymers. *This work inspires Thrusts 1 and 2, which emphasize multiscale modeling to advance soft materials design.*

Future Research Plans

1. Machine Learning for Topologically Complex Soft Materials Design

Topologically complex soft materials, such as those with branched, star, and network architectures, exhibit unique mechanical, transport, and functional properties unattainable with linear chain topologies[16]. However, designing these materials remains challenging, as existing methods struggle to capture multiscale topological effects on macroscopic behavior[17]. *To address this, we will develop machine learning frameworks that incorporate soft material topology to accelerate discovery of new structures with tailored properties (Figure 2).*

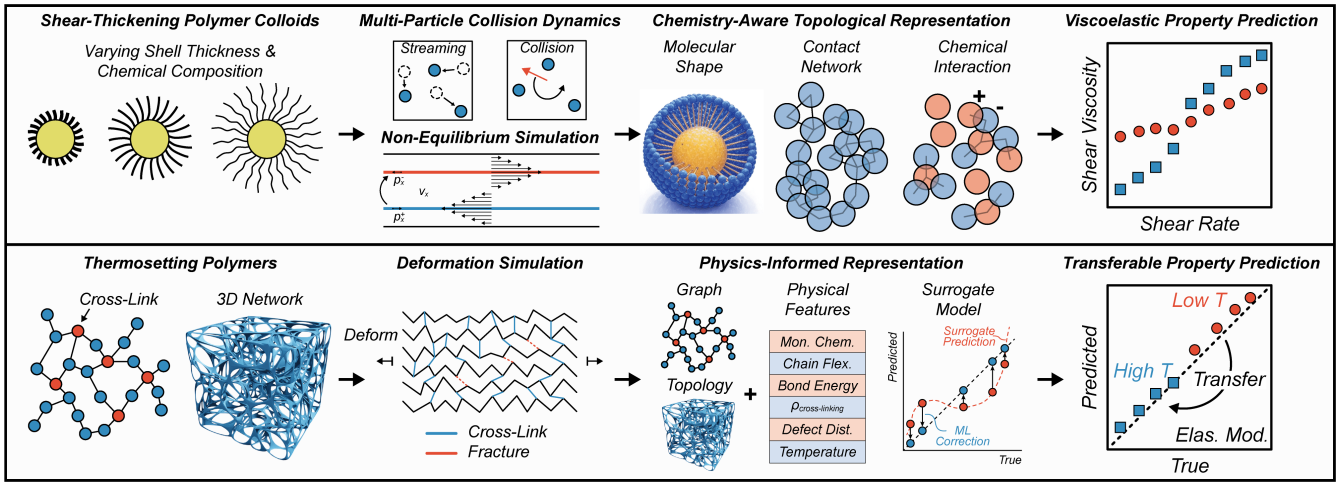

Figure 2: Soft materials data representation and machine learning workflows. (*Top*) *Multiscale topological representation for shear-thickening soft materials.* Microgels are modeled over ranges of volume fractions, shell thicknesses, and chemical compositions, from which topological analysis (e.g., persistent homology) extracts features for machine learning models to predict nonlinear rheology. (*Bottom*) *Physics-informed representation for thermosets.* Reactions are modeled using kinetic theory and coarse-grained molecular dynamics to capture cure-dependent network evolution, while physics-informed neural networks incorporate chemical specificity, topological descriptors, and scaling laws to predict mechanical properties under varied conditions.

1.1 Topological Representations for Shear-Thickening Soft Materials Design

Motivation: Shear-thickening in soft polymer colloids, such as poly(N-isopropylacrylamide) (PNIPAM) microgel suspensions[18], emerges from a complex interplay of frictional jamming, hydroclustering, and thermo-responsive deformation[19]. This behavior enables adaptive fluid-to-solid transitions, offering potential for applications including flexible body armor and vibration dampers[20,21]. However, achieving precise control over the onset and magnitude of shear-thickening remains difficult, as current methods depend heavily on trial-and-error experiments that are often confined to limited parameter ranges (e.g., particle softness and concentration)[22]. Furthermore, the hierarchical topology of colloidal networks, which plays a crucial role in driving shear-thickening, has been investigated only at a coarse level and typically lacks detailed chemical specificity in existing models[17]. To address this, *we aim to develop a chemistry-aware topological representation integrating multiscale structure and chemical data to predict nonlinear rheology from colloidal microstructures.*

Approach: *In the short term*, we will investigate thermo-responsive microgels, specifically PNIPAM, with tunable shell chemistry (e.g., incorporating co-monomers to adjust hydrophilicity), using coarse-grained molecular dynamics and multi-particle collision dynamics simulations to model temperature-dependent swelling under varying shear conditions. These simulations will monitor the evolution of frictional contacts and network formation across a range of particle volume fractions and shell chemical compositions. Drawing on my expertise in topological data analysis[7], we will apply persistent homology and the Mapper algorithm[23] to extract chemistry-dependent topological features from interaction graphs and molecular shapes, condensing them into low-dimensional shape descriptors that reflect hierarchical structures. Interpretable models, such as

random forests enhanced with SHAP analysis, will then correlate multiscale topological features with shear-thickening behavior, identifying key structural motifs that may influence rheological responses. *In the long term*, we aim to elucidate how microgel structure, chemistry, and concentration influence viscosity under shear, resolving many-to-one relationships where diverse microstructures produce similar rheological outcomes. This framework will be extended to other soft colloidal systems, including shape-memory polymers, by adapting coarse-grained models to capture reversible network dynamics.

Impact: Optimize design principles for shear-thickening fluids, advancing applications in impact-resistant protective gear, flexible armor systems, and adaptive soft robotics.

1.2 Physics-Informed Representations for Thermoset Design under Dynamic Conditions

Motivation: Thermosets, such as epoxy resins, are essential materials prized for their mechanical strength, thermal resistance, and dimensional stability, making them critical for aerospace, automotive, and electronics applications[24]. A significant challenge arises in designing these materials to perform reliably in dynamic environments characterized by fluctuating temperatures and pressures, a task complicated by the extensive chemical diversity of thermosets—including variations in monomers, curing agents, and curing profiles—which vastly expands the design space[25]. This challenge is further intensified by the scarcity of comprehensive datasets, as experimental data for specific formulations are often limited, expensive to generate, and confined to narrow conditions[25]. Existing data-driven models struggle to effectively integrate network topology, reaction kinetics, and dynamic operating conditions, limiting predictive transferability across diverse scenarios[26]. To address these limitations, *we will develop a physics-informed framework integrating environment-dependent interactions, network evolution, and scaling laws for transferable thermoset property predictions under varied conditions*.

Approach: *In the short term*, we will investigate epoxy–amine systems, focusing on the DGEBA (diglycidyl ether of bisphenol A)–diamine benchmark pair, valued for its industrial relevance and well-characterized curing kinetics[27]. Kinetic modeling will track network formation and topology evolution under varying temperatures and stoichiometries, optimized for computational tractability to balance accuracy and efficiency. These insights will guide coarse-grained models to explore connections between network topology and key properties such as glass transition temperature (T_g), elastic modulus, and temperature-dependent responses. Drawing on my expertise in physics-informed neural networks[6], we will develop models that integrate physical features (e.g., chain flexibility, cross-link density), topological descriptors, and surrogate models grounded in scaling laws (e.g., rubber elasticity theory for modulus above T_g), aiming to support transferable property predictions across different conditions. *In the long term*, we will extend this framework to alternative amine hardeners, resin blends, and other thermosets (e.g., cyanate esters, bismaleimides, vitrimers)[28–30], employing transfer learning to adapt latent representations derived from epoxy–amine data. This process will address potential challenges in generalizing to systems with distinct chemical mechanisms, such as reversible bonds in vitrimers, while performance will be benchmarked against literature datasets and, where feasible, validated through collaborative experimental studies under diverse curing and environmental conditions.

Impact: Establish a processing–structure–property mapping for thermosets under dynamic environments, accelerating the design of advanced aerospace composites and automotive materials.

2. Physics-Informed Closed-Loop Discovery of Soft Materials for Energy and Sustainability

Soft materials are key to clean energy and sustainable manufacturing. Traditional discovery methods rely on slow, resource-intensive experiments that explore limited design spaces. Generative artificial intelligence (AI) explores vast design spaces but often yields synthetically inaccessible or poorly scalable candidates[31]. *We will develop a physics-informed closed-loop framework combining data-driven generation and heterogeneous data sources to design high-performing, synthesizable, and economically viable soft materials (Figure 3).*

2.1 Polymeric Membranes for Lithium Extraction from Seawater

Motivation: The transition to a clean energy economy relies on lithium, a vital battery material, though its extraction through traditional mining and brine methods causes significant environmental harm and is geo-

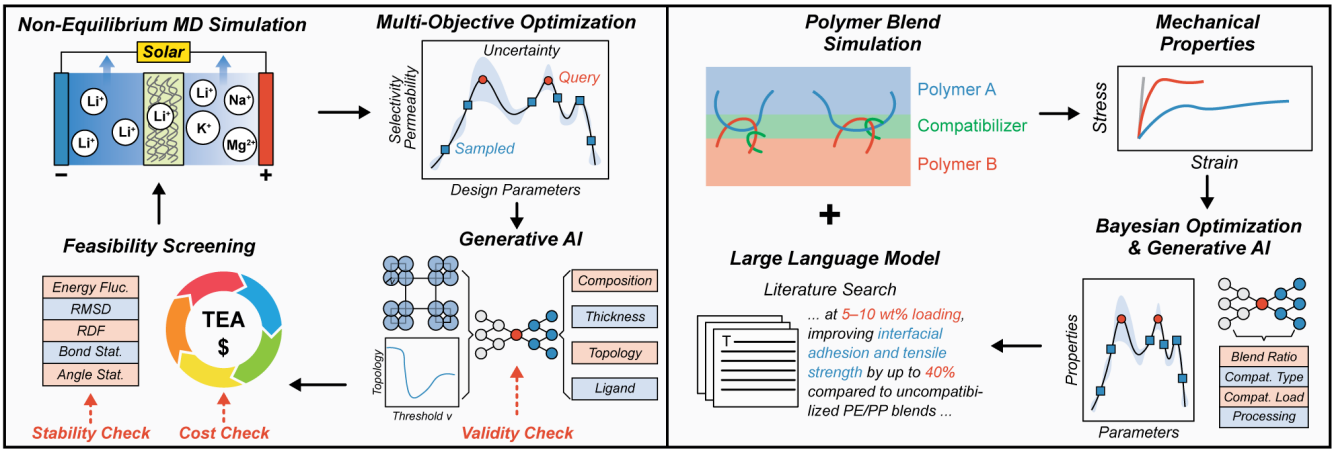

Figure 3: Physics-informed closed-loop learning framework for soft materials discovery. (*Left*) *Polymeric membranes for lithium extraction from seawater.* Molecular dynamics simulations and physical constraints inform surrogate models to optimize membrane chemistry and topology, enhancing Li^+ selectivity, permeability, and durability. (*Right*) *Recyclable polymer blends.* Blend ratios, compatibilizer strategies, and interfacial mechanics are integrated into surrogate models, combined with literature-mined data in optimization loops, to balance flexibility, toughness, and recyclability.

graphically limited[32]. Seawater offers a vast, potentially inexhaustible lithium reserve, yet selective extraction is highly challenging due to its ultra-low concentration (0.1–0.2 ppm) and the presence of competing ions (e.g., Na^+, Mg^{2+}, Ca^{2+}) at much higher levels[33]. Polymeric membranes present a sustainable alternative, but current designs struggle with trade-offs between Li^+ permeability, selectivity, and durability, particularly under saline conditions[34]. These challenges are exacerbated by a vast design space (e.g., chemical functionality and polymer topology) where experimental progress is slow due to costly testing, and simulations, often focusing on idealized scenarios like single-ion transport, have only coarsely explored complex ion-coupling effects[35,36]. To address these challenges, *we will develop a closed-loop framework to optimize Li^+ permeability, selectivity, and durability in polymeric membranes under operational constraints.*

Approach: *In the short term*, we will target poly(ether sulfone) (PES), a chemically stable and processable filtration polymer with tunable functionalization (e.g., sulfonation or crown ether grafting) to enhance Li^+ coordination while preserving durability[35]. Atomistic molecular dynamics will model Li^+ interactions with polymeric membranes under mixed-ion conditions (Na^+, Mg^{2+}, Ca^{2+}) at elevated Li^+ concentrations, mimicking industrial preconcentration processes[37]. A scaling study across concentration gradients will aim to assess the applicability of these models to dilute seawater conditions and explore interactions among competing ions. *Subsequently*, simulation-derived features (e.g., network descriptors, ion coordination numbers) will train a neural network to predict Li^+ selectivity, permeability, and mechanical properties. These predictions will drive a Bayesian optimization process to propose novel polymeric membrane variants, focusing on design improvements based on simulated trends. *In the long term*, we will extend the framework to non-equilibrium atomistic molecular dynamics under applied electric fields to model ion transport and selectivity relevant to electrodialysis, noting challenges such as limited timescales and complex electrode-membrane interfaces[38]. Supported by potential techno-economic analysis collaborations focusing on cost and energy efficiency, this approach seeks to bridge molecular design to process performance, fostering scalable membrane solutions for seawater lithium extraction.

Impact: Advance understanding of how polymer chemistry and topology govern ion selectivity and transport, while designing durable, high-performing membranes to enable scalable lithium extraction for clean energy.

2.2 Recyclable Polymer Blends with Optimized Mechanical Performance

Motivation: The global plastic waste crisis urgently requires scalable recycling strategies[39]. Mechanical

recycling of mixed polymers, such as polyethylene (PE) and polypropylene (PP), often results in brittle materials with reduced tensile strength and flexibility, driven by thermodynamic incompatibility, phase separation, and poor interfacial adhesion[40]. This challenge is compounded by a complex design space encompassing blend ratios, compatibilizers (e.g., block copolymers or reactive agents), and processing parameters, which complicates optimization efforts[41,42]. Furthermore, the effects of multi-cycle reprocessing (e.g., chain scission, oxidative degradation, and interfacial coarsening) remain inadequately studied in simulations, limiting insights into long-term recyclability[43]. To address this, *we will integrate simulations with large language models to rationally design recyclable polymer blends with optimized mechanical properties.*

Approach: *Initially*, we will focus on polyethylene/polypropylene (PE/PP) blends, common in recycled streams, and employ compatibilizers such as copolymers and emerging vitrimeric additives to reduce interfacial tension and improve adhesion[41,44]. We will vary blend ratios, compatibilizer species, and loadings, using atomistic molecular dynamics to model interfacial mechanics under uniaxial deformation. Multi-cycle reprocessing degradation will be approximated with heating–cooling–shearing protocols and proxy models, simulating reduced chain lengths and imposed defects to capture chain scission and interfacial coarsening trends. *Subsequently*, a large language model (e.g., a fine-tuned BERT variant) will extract structure–property relationships from polymer literature, though challenges like inconsistent data quality and potential bias in text interpretation may arise, requiring iterative refinement and computational resource management. A neural network surrogate will predict modulus, toughness, and recyclability across cycles, driving a multi-objective Bayesian optimization loop to map Pareto trade-off frontiers and balance these metrics. *In the long term*, we aim to extend this framework to higher-order blends (e.g., PE/PP/PET ternaries), addressing interfacial coarsening, uneven phase distribution, and accelerated degradation, potentially enhancing durability with optimized compatibilizer and processing strategies.

Impact: Provide insights into compatibilizer and interfacial topology control to balance strength, ductility, and recyclability in polymer blends, enabling durable materials for sustainable packaging and automotive sectors.

3. Scalable Autonomous Materials Discovery

The next frontier in soft materials discovery lies not in a single model, but in a scalable system that continuously integrates simulations, AI, and experiments. Existing closed-loop frameworks are often synchronous and siloed, failing to capture the multi-source nature of real-world discovery. *To bridge this gap, we will develop computational systems to support asynchronous decision-making and collective intelligence, enabling open-source platforms for exploration under uncertainty in distributed resources (Figure 4).*

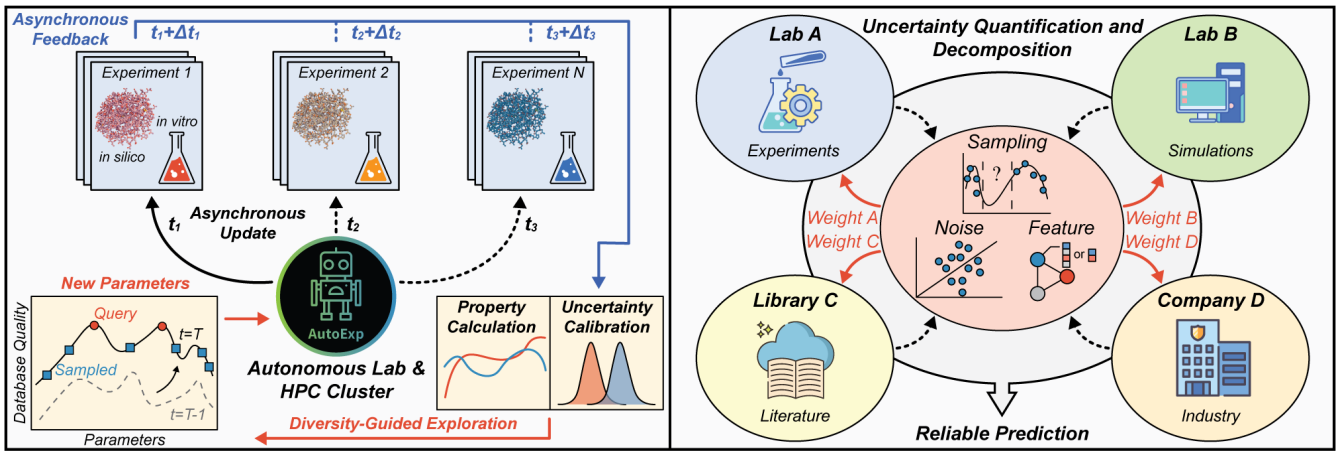

Figure 4: Scalable autonomous discovery workflows. (*Left*) `AutoExp`, an asynchronous closed-loop learning platform that integrates multi-fidelity simulations, Bayesian optimization, and experimental feedback to accelerate materials exploration. (*Right*) Multi-modal polymer data fusion, where heterogeneous sources (experiments, simulations, literature) are embedded into probabilistic models yielding calibrated predictions, decomposed uncertainties, and actionable data-acquisition guidance.

3.1 Scalable Asynchronous Platform for Autonomous Data Generation

Motivation: Materials discovery faces significant barriers due to the high costs and extended timelines of experimental characterization[45]. Closed-loop learning can guide experiments toward optimal candidates, but synchronous methods—where computation remains idle awaiting results—leave laboratory and computational resources underutilized. Asynchronous strategies, incorporating multi-fidelity modeling[46,47], mitigate downtime yet lack seamless integration with soft materials experiments and simulation pipelines, alongside insufficient uncertainty calibration. *We will develop* `AutoExp`*, an automated platform for asynchronous closed-loop learning, integrating computational and experimental workflows to streamline soft materials discovery.*

Approach: *In the short term*, development of a multi-fidelity Bayesian optimization (MFBO) framework for `AutoExp` will address the limitation of fixed fidelity correlations in standard MFBO, which struggle with complex, non-linear trends across materials chemistries and processing conditions. Employing heteroscedastic Gaussian processes with deep kernel learning will capture adaptive fidelity correlations, enhancing prediction robustness amid varying data quality. A calibration module, leveraging uncertainty quantification expertise[14], will guide high-fidelity evaluations (e.g., atomistic simulations) using low-cost surrogates (e.g., coarse-grained models), distinguishing aleatoric (inherent noise) and epistemic (knowledge gaps) uncertainties via Bayesian recalibration and ensembles. The `AutoExp` queueing system will enable asynchronous decision-making with task prioritization, interfacing with `LAMMPS`, `HOOMD-blue`, and `OpenMM`. Validation will use case studies from Thrusts 1 and 2 to show accelerated exploration. Challenges include harmonizing heterogeneous data sources while preserving fidelity, which may demand advanced data alignment techniques. *In the long term*, `AutoExp` will integrate with autonomous platforms and high-throughput resources (e.g., Aurora at Argonne National Laboratory), expanding materials discovery despite integration hurdles.

Impact: Deliver a platform unifying simulation and experiment in a scalable, uncertainty-calibrated closed-loop framework, transforming materials discovery from ad hoc trial-and-error to systematic, continuous learning.

3.2 Uncertainty Quantification in Multi-Modal Polymer Data Fusion

Motivation: Effective polymer property prediction requires integrating diverse data from experiments, simulations, and literature. Conventional methods, such as data concatenation, often introduce spurious correlations and overlook source-specific uncertainties, leading to unreliable predictions, especially with missing data or across varying chemical spaces. These models may achieve high test accuracy on average but falter under different experimental protocols or data distributions. Uncertainty quantification offers a pathway to enhance reliability[48], yet challenges remain in attributing uncertainties to data sources and adapting to distribution shifts across laboratories. *We will develop a theory-driven fusion framework that calibrates uncertainties, attributes them to sources, and guides data acquisition for robust polymer property predictions.*

Approach: *In the short term*, we will predict the glass transition temperature (T_g), essential for polymer stability and processability, by integrating SMILES/BigSMILES representations[49], established databases[50], and text-mined literature features. Modality-specific encoders—graph neural networks for structural data, probabilistic encoders for metadata (e.g., molecular weight distributions), and transformers for literature—will feed into a hierarchical probabilistic model with cross-attention mechanisms to fuse sources and handle missing data through imputation or masking. This architecture explicitly learns the conditional informativeness of each modality, outputting T_g estimates with uncertainty decomposed into aleatoric, epistemic, and protocol-related components. Validation against molecular simulations and experimental benchmarks will ensure reliability, though challenges in cross-modal alignment and computational scaling of transformers may require iterative refinement. *In the long term*, we aim to extend domain adaptation techniques to address biased datasets and apply the framework to rheological properties like shear-thickening onset, delivering an open-source toolkit with calibrated predictions and actionable guidance for protocol standardization and chemistry exploration.

Impact: Establish a framework for uncertainty-aware polymer informatics, fostering reliable predictions, transparent uncertainty attribution, and informed strategies for advancing materials design and discovery.

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