
Professional Certificate in Materials Design with AI Optimization

Advanced Materials Synthesis

Advanced Materials Synthesis lies at the intersection of chemistry, physics, engineering, and increasingly, artificial intelligence. Mastery of the terminology used in this field is essential for clear communication, efficient literature review, and effective collaboration across disciplines. The following glossary-style exposition presents the most frequently encountered terms, organized thematically, and illustrates each with practical examples, typical applications, and common challenges. Where appropriate, the role of AI-driven optimization is highlighted to show how modern computational tools accelerate discovery and scale-up.

1. Synthesis Pathways

Sol-gel process – A wet-chemical route that converts molecular precursors, usually metal alkoxides, into a colloidal suspension (sol) and then into a three-dimensional network (gel). The gel is subsequently dried and heat-treated to yield oxide ceramics or glasses. Example: Synthesis of titania (TiO₂) nanoparticles for photocatalytic water splitting. Application: Production of transparent conductive oxides for display technologies. Challenge: Controlling shrinkage and crack formation during drying, which can compromise mechanical integrity.

Hydrothermal synthesis – Crystallization of materials in sealed, high-pressure aqueous environments at temperatures typically between 150 °C and 350 °C. The method enables growth of single-crystalline nanostructures that are difficult to obtain by conventional routes. Example: Growth of ZnO nanorods on flexible polymer substrates for piezoelectric sensors. Application: Fabrication of battery cathode materials such as LiFePO₄ with enhanced crystallinity. Challenge: Precise control of supersaturation and nucleation kinetics; scaling up autoclave operations while maintaining uniformity.

Chemical Vapor Deposition (CVD) – Deposition of thin films from vapor-phase precursors that react or decompose on a heated substrate. Variants include low-pressure CVD, plasma-enhanced CVD, and metal-organic CVD. Example: Deposition of silicon carbide (SiC) coatings on turbine blades for high-temperature protection. Application: Manufacturing of graphene layers on copper foils for electronic devices. Challenge: Managing precursor toxicity, ensuring conformal coverage over complex topographies, and minimizing defect density.

Atomic Layer Deposition (ALD) – A self-limiting, sequential surface reaction technique that deposits one atomic layer per cycle, yielding unparalleled thickness control and uniformity even on high-aspect-ratio structures. Example: Alumina (Al₂O₃) passivation layers on perovskite solar cells to improve stability. Application: High-k dielectric layers in advanced CMOS transistors. Challenge: Low throughput compared with CVD, requiring careful optimization of precursor pulse times and purge steps.

Mechanochemical synthesis – Solid-state reactions induced by mechanical energy, typically using ball-mill grinding. The high energy impacts create defects and facilitate diffusion, enabling synthesis of metastable

phases at relatively low temperatures. Example: Production of nanocrystalline nickel-aluminum alloy powders for additive manufacturing feedstocks. Application: Synthesis of lithium-ion battery cathode materials such as LiMn_2O_4 without high-temperature calcination. Challenge: Controlling particle size distribution and preventing contamination from milling media.

Spark Plasma Sintering (SPS) – A rapid consolidation technique that applies pulsed electric current and uniaxial pressure to powders, achieving high densities in minutes. The process leverages Joule heating and plasma formation at particle contacts. Example: Densification of magnesium-based composites for lightweight aerospace components. Application: Production of thermoelectric ceramics with fine grain structures that preserve low thermal conductivity. Challenge: Managing temperature gradients, avoiding localized overheating, and ensuring reproducibility across large batches.

Electrochemical deposition (ECD) – Deposition of metals or alloys onto conductive substrates by applying a potential in an electrolyte solution. The method is widely used for plating, coating, and nanostructure growth. Example: Electrodeposition of copper interconnects in printed circuit board fabrication. Application: Formation of metallic nanowire arrays for flexible electronics. Challenge: Achieving uniform deposition over large areas, mitigating dendrite formation, and controlling impurity incorporation.

Solvothermal synthesis – Similar to hydrothermal methods but using non-aqueous solvents (e.g., Ethanol, ethylene glycol). The approach can tailor solvent-mediated interactions, leading to unique morphologies. Example: Synthesis of bismuth oxyhalide nanosheets in ethylene glycol for photocatalytic degradation of organics. Application: Production of metal-organic frameworks (MOFs) with solvent-dependent pore architectures. Challenge: Selecting solvents with appropriate boiling points and reactivity while ensuring safe handling.

Microwave-assisted synthesis – Utilization of microwave irradiation to heat reaction mixtures rapidly and uniformly, often reducing synthesis times from hours to minutes. Example: Rapid formation of carbon quantum dots from glucose precursors. Application: High-throughput synthesis of catalyst nanoparticles for screening libraries. Challenge: Penetration depth limitations for large volumes, and the need for microwave-transparent reaction vessels.

Laser-induced forward transfer (LIFT) – A direct-write technique where a laser pulse ablates material from a donor substrate and deposits it onto a receiver, enabling patterning of functional inks. Example: Deposition of conductive silver nanoparticle inks onto flexible polymer films for printed electronics. Application: Fabrication of micro-LED arrays for display technologies. Challenge: Controlling droplet size and avoiding thermal damage to sensitive substrates.

2. Materials Classes and Structural Descriptors

Metal-Organic Frameworks (MOFs) – Crystalline porous materials composed of metal nodes connected by organic linkers, forming extended networks with tunable pore sizes. Example: UiO-66 zirconium-based MOF for gas storage. Application: Catalytic supports for selective hydrogenation reactions. Challenge: Scalability of synthesis, solvent recovery, and post-synthetic modification stability.

Perovskites – Compounds with the general formula ABX_3 , where A and B are cations and X is an anion (often

halide or oxide). The structure supports a wide range of electronic and optical properties. Example: Methylammonium lead iodide (MAPbI₃) for solar cells. Application: Light-emitting diodes (LEDs) with high color purity. Challenge: Moisture sensitivity, lead toxicity, and long-term stability under operational conditions.

High-Entropy Alloys (HEAs) – Multi-principal element alloys that contain five or more elements in near-equimolar proportions, leading to high configurational entropy and often superior mechanical properties. Example: CoCrFeMnNi alloy for cryogenic applications. Application: Wear-resistant coatings for cutting tools. Challenge: Predicting phase stability, controlling segregation during solidification, and optimizing processing routes.

Two-Dimensional (2D) Materials – Atomically thin layers with strong in-plane bonding and weak out-of-plane interactions, such as graphene, transition-metal dichalcogenides (TMDs), and phosphorene. Example: MoS₂ monolayers for field-effect transistors. Application: Flexible photodetectors and strain sensors. Challenge: Large-area synthesis, layer-number control, and integration with existing device architectures.

Nanocomposites – Materials comprising a matrix (polymeric, metallic, or ceramic) reinforced with nanoscale fillers (nanoparticles, nanowires, nanosheets). The synergy between phases can enhance mechanical, electrical, or thermal performance. Example: Graphene-reinforced epoxy for aerospace structural components. Application: Thermal interface materials with high conductivity and low thickness. Challenge: Achieving uniform dispersion, preventing agglomeration, and maintaining interfacial bonding during processing.

Amorphous Alloys (Metallic Glasses) – Non-crystalline alloys formed by rapid quenching that suppresses crystallization, resulting in high strength and elastic limit. Example: Zr-based bulk metallic glass for biomedical implants. Application: Magnetic soft materials for transformer cores. Challenge: Limited thickness achievable by conventional casting, susceptibility to shear banding, and difficulty in tailoring composition for specific properties.

Quantum Dots (QDs) – Semiconductor nanocrystals with size-dependent band gaps, enabling tunable emission wavelengths. Example: CdSe/ZnS core-shell quantum dots for display backlighting. Application: Bio-imaging agents with high photostability. Challenge: Toxicity of heavy-metal constituents, surface trap states, and batch-to-batch reproducibility.

3. Process Variables and Control Parameters

Precursor purity – The chemical purity of starting materials, which directly influences defect concentration, impurity phases, and overall material performance. Practical tip: Use high-purity metal salts (≥99.999%) For semiconductor synthesis to minimize carrier recombination centers.

Stoichiometry – The precise ratio of elements in a compound. Deviations can lead to secondary phases, vacancy formation, or altered electronic structure. Example: Slight excess of lithium in LiFePO₄ synthesis improves rate capability by reducing Li-vacancy concentration.

Temperature ramp rate – The speed at which temperature is increased during heat treatment. Fast ramps can suppress grain growth, while slow ramps promote equilibrium phase formation. Challenge: Balancing rapid processing with avoidance of thermal shock that may cause cracking.

Atmosphere composition – The gases present during synthesis (e.g., Inert, reducing, oxidizing). The atmosphere can dictate oxidation state, volatilization, and surface chemistry. Example: Argon atmosphere during CVD of silicon nitride to prevent oxygen incorporation.

Pressure – Particularly relevant in hydrothermal, solvothermal, and vapor-phase processes. Elevated pressure can increase solubility, alter reaction pathways, and affect nucleation density. Example: 10 MPa pressure in hydrothermal synthesis of BaTiO₃ yields higher dielectric constants.

pH – In aqueous syntheses, the solution pH governs hydrolysis rates, surface charge, and precipitation behavior. Example: Adjusting pH to 9 during sol-gel synthesis of silica promotes faster condensation.

Reaction time – Duration of exposure to synthesis conditions. Longer times can enhance crystallinity but may also promote particle agglomeration. Challenge: Determining optimal time that balances phase purity with throughput.

Particle size distribution (PSD) – A statistical description of particle sizes within a batch. Narrow PSD is often required for uniform sintering, consistent optical properties, and reliable performance. Tool: Dynamic light scattering (DLS) for rapid PSD assessment.

Surface energy – The excess energy associated with the surface of a material. Surface energy influences nucleation, wetting, and adhesion. Application: Tailoring surface energy of catalyst supports to improve metal nanoparticle dispersion.

4. Characterization Techniques (Vocabulary)

X-ray Diffraction (XRD) – A diffraction technique that provides crystallographic information such as phase identification, lattice parameters, and crystallite size. Key term: Rietveld refinement – A method for quantitative phase analysis and structure refinement from powder diffraction data.

Scanning Electron Microscopy (SEM) – Imaging technique that uses a focused electron beam to generate high-resolution surface topography and composition contrast. Key term: Backscattered electron (BSE) imaging for atomic number contrast.

Transmission Electron Microscopy (TEM) – Provides atomic-scale imaging and diffraction; essential for assessing nanostructure morphology, defects, and lattice fringes. Key term: Selected area electron diffraction (SAED) for local crystallography.

Energy-Dispersive X-ray Spectroscopy (EDS) – Elemental analysis attached to SEM/TEM, yielding qualitative and semi-quantitative compositional maps. Note: Detection limits typically around 0.1 Wt%.

Raman Spectroscopy – Vibrational spectroscopy that probes molecular and lattice vibrations; useful for identifying carbon allotropes, phase transitions, and stress states. Key term: G-band and D-band for carbon

materials.

Fourier-Transform Infrared Spectroscopy (FTIR) – Identifies functional groups and bonding environments, especially in organic-inorganic hybrids and MOFs. Application: Monitoring ligand removal in post-synthetic MOF activation.

X-ray Photoelectron Spectroscopy (XPS) – Surface-sensitive technique that provides elemental composition, oxidation states, and chemical environment within the top ~10 nm. Key term: Binding energy shift for detecting charge transfer.

Brunauer-Emmett-Teller (BET) Analysis – Determines specific surface area via gas adsorption; essential for catalysts, adsorbents, and porous materials. Key term: Langmuir isotherm for monolayer adsorption assessment.

Thermogravimetric Analysis (TGA) – Measures weight change as a function of temperature; used to evaluate decomposition, oxidation, and moisture content. Example: Quantifying organic template removal in sol-gel derived ceramics.

Differential Scanning Calorimetry (DSC) – Detects endothermic and exothermic events, providing insight into phase transitions, glass transition temperature (T_g), and crystallization kinetics. Application: Identifying the crystallization temperature of metallic glasses.

5. AI-Driven Optimization Concepts

Surrogate Modeling – Construction of an inexpensive predictive model (e.g., Gaussian process, neural network) that approximates the behavior of a complex, computationally expensive simulation or experiment. Use case: Predicting the yield of a nanoparticle synthesis as a function of temperature, precursor concentration, and reaction time, thereby reducing the number of actual experiments.

Bayesian Optimization – An iterative strategy that uses a surrogate model and an acquisition function to select the next experimental condition that maximizes expected improvement. Benefit: Efficient exploration of high-dimensional synthesis spaces with limited experimental budget.

Design of Experiments (DoE) Integration – Combining classical factorial or response-surface designs with AI algorithms to refine parameter spaces and accelerate convergence toward optimal conditions. Example: Starting with a fractional factorial design, then feeding results into a Bayesian optimizer to fine-tune catalyst composition.

Reinforcement Learning (RL) – A machine-learning paradigm where an agent learns to make sequential decisions (e.g., Adjusting temperature, adding reagents) by receiving rewards based on measured material properties. Application: Autonomous laboratory robots that iteratively adjust synthesis parameters to achieve target bandgap values in perovskite films.

Generative Models – Algorithms such as variational autoencoders (VAEs) or generative adversarial networks (GANs) that can generate new material compositions or synthesis recipes from learned latent spaces. Use case: Proposing novel MOF linkers that satisfy both pore size and thermal stability constraints.

Feature Engineering – The process of extracting meaningful descriptors (e.G., Atomic radius, electronegativity, coordination number) from raw data to improve model performance. In materials synthesis, features may include processing parameters, precursor properties, and thermodynamic data. Tip: Include both numerical (temperature, pressure) and categorical (solvent type, catalyst) features to capture complex interactions.

Active Learning – A strategy where the model actively selects the most informative experiments to perform next, based on current uncertainty. Benefit: Rapidly reduces model error with fewer experiments, ideal for costly high-throughput synthesis campaigns.

High-Throughput Experimentation (HTE) – Parallel synthesis and testing of large libraries of materials using automated platforms. AI algorithms analyze the resulting data streams to identify promising candidates. Example: 96-Well plate synthesis of alloy compositions for rapid screening of corrosion resistance.

Data-Driven Materials Design – Leveraging large databases (e.G., Materials Project, OQMD) and machine learning to predict property trends, guide synthesis routes, and identify gaps in existing knowledge. Challenge: Ensuring data quality, handling missing values, and reconciling disparate measurement standards across literature.

Uncertainty Quantification (UQ) – Assessing the confidence in model predictions, often expressed as confidence intervals or probability distributions. UQ informs decision-making, especially when selecting synthesis conditions that may be near safety limits. Tool: Monte Carlo sampling of model parameters to propagate uncertainty through to predicted material performance.

6. Process Integration and Scale-Up Vocabulary

Continuous Flow Synthesis – A paradigm where reactants are continuously fed into a reactor (often micro- or meso-scale) and products are collected downstream, enabling precise control over residence time and temperature. Example: Continuous hydrothermal flow synthesis of TiO₂ nanorods for large-scale pigment production. Advantage: Improved reproducibility and easier scale-up compared with batch processes.

Process Analytical Technology (PAT) – Real-time monitoring tools (e.G., Inline spectroscopy, calorimetry) that provide feedback for closed-loop control of synthesis. Implementation: In-line Raman monitoring of polymerization to detect monomer conversion and adjust feed rates automatically.

Scale-up Factor (SUF) – The ratio of product output in a pilot or industrial plant to that obtained in a laboratory-scale experiment. SUF is used to evaluate feasibility and identify scaling bottlenecks. Consideration: Heat and mass transfer limitations often become dominant at higher SUF values.

Batch-to-Continuous Transition – The process of converting a traditionally batch-based synthesis into a continuous operation, typically to increase throughput and reduce variability. Key step: Designing reactors that maintain the same residence time distribution as the batch process while allowing for modular expansion.

Thermal Management – Strategies for controlling heat flow in synthesis reactors, crucial for exothermic or

highly temperature-sensitive reactions. Technique: Use of heat exchangers and active cooling loops in large-scale CVD reactors to prevent substrate overheating.

Material Handling Safety – Protocols for safe transport, storage, and disposal of hazardous precursors (e.G., Metal alkoxides, organometallics). Standard: Compliance with OSHA and REACH regulations, implementation of glove-box or fume-hood environments for air-sensitive materials.

Life-Cycle Assessment (LCA) – Evaluation of the environmental impact of a material from raw-material extraction through synthesis, use, and end-of-life. AI can assist by integrating process data and predicting emissions. Application: Comparing the carbon footprint of sol-gel versus CVD routes for thin-film production.

7. Terminology Specific to AI-Optimized Materials Design

Descriptor – A numerical representation of a material or process characteristic used as input for machine-learning models. Descriptors can be simple (e.G., Temperature) or complex (e.G., Graph-based representation of a crystal structure). Example: Using the partial radial distribution function as a descriptor for amorphous alloy structure.

Latent Space – An abstract, reduced-dimensional space learned by generative models where similar materials cluster together. Navigation in latent space can reveal unexplored compositions with desired properties. Practice: Interpolating between two known high-performance catalysts in latent space to propose intermediate compositions.

Transfer Learning – Reusing a pre-trained model (often on a large, generic dataset) as a starting point for a more specific task, thereby reducing the amount of required training data. Scenario: Fine-tuning a neural network trained on bulk alloy data to predict thin-film stress in sputtered coatings.

Ensemble Modeling – Combining predictions from multiple models (e.G., Random forest, gradient boosting, neural network) to improve robustness and reduce overfitting. Benefit: Provides more reliable uncertainty estimates for synthesis optimization.

Explainable AI (XAI) – Techniques that make model decisions interpretable, such as SHAP values or feature importance plots. XAI helps scientists understand why a particular synthesis condition is predicted to be optimal. Use case: Identifying that solvent polarity, rather than temperature, drives the morphology change in a solvothermal synthesis.

Hyperparameter Tuning – The process of selecting optimal settings for model parameters (e.G., Learning rate, number of layers) that are not learned during training. Automated tools like Bayesian optimization can perform hyperparameter tuning efficiently. Impact: Proper tuning can dramatically improve the predictive accuracy of surrogate models for synthesis outcomes.

Data Augmentation – Generating synthetic data points (e.G., By adding noise or applying physical constraints) to expand limited experimental datasets, enhancing model training. Application: Augmenting a small set of XRD patterns with simulated variations to train a classifier for phase identification.

Cross-Validation – A statistical method for evaluating model performance by partitioning data into training and validation subsets multiple times. Ensures that models generalize well to unseen synthesis conditions. Best practice: Use k-fold cross-validation with stratified sampling when dealing with imbalanced datasets (e.G., Few successful synthesis runs among many failures).

Domain Knowledge Integration – Incorporating expert rules, thermodynamic constraints, or mechanistic insights into AI models to guide learning and avoid physically impossible predictions. Example: Enforcing charge-balance constraints when proposing new alloy compositions.

8. Common Challenges in Advanced Synthesis and AI Optimization

Reproducibility – Even minor variations in precursor quality, ambient humidity, or equipment calibration can lead to divergent results. AI models trained on inconsistent data may learn spurious correlations. Mitigation: Implement rigorous standard operating procedures (SOPs) and record all metadata (e.G., Batch numbers, instrument settings) for each experiment.

Data Scarcity – High-fidelity synthesis experiments are often time- and resource-intensive, leading to limited datasets. Small datasets increase the risk of overfitting and reduce confidence in model predictions. Strategy: Combine experimental data with physics-based simulations to enrich the training set, and employ active learning to prioritize informative experiments.

Complex Interdependencies – Synthesis parameters frequently interact in non-linear ways (e.G., Temperature influences solvent evaporation, which in turn affects nucleation). Simple linear models fail to capture these effects. Solution: Use non-linear models such as Gaussian processes with kernel functions that can model interactions, or deep neural networks with sufficient capacity.

Safety Constraints – Some optimal conditions suggested by AI (e.G., High pressure, reactive gases) may be unsafe or impractical in a laboratory setting. Approach: Encode safety limits as hard constraints within the optimization algorithm, or use penalty functions to discourage unsafe proposals.

Interpretability vs. Performance – Highly accurate models (e.G., Deep neural networks) may be opaque, making it difficult for scientists to trust or act on the recommendations. Balance: Deploy hybrid models that combine interpretable linear components with flexible non-linear parts, and use XAI tools to extract insights.

Integration with Existing Workflows – Many labs have entrenched experimental protocols and equipment. Introducing AI-driven optimization requires software-hardware interfacing, data pipelines, and staff training. Recommendation: Start with a pilot project that automates a single step (e.G., Temperature ramp) and gradually expand to full workflow integration.

Computational Resource Limits – Training large models or running high-fidelity simulations can demand substantial CPU/GPU resources, which may not be readily available. Workaround: Use cloud-based services for on-demand scaling, or employ model compression techniques (e.G., Pruning, quantization) for faster inference.

Model Drift – Over time, as new data are collected, the underlying process may evolve (e.G., Equipment

wear, changes in raw material batches), causing the AI model's predictions to become less accurate. Maintenance: Schedule periodic retraining and validation cycles, and monitor performance metrics continuously.

Regulatory and Ethical Considerations – When AI designs materials that may have environmental or health impacts (e.G., Lead-based perovskites), responsible stewardship is required. Action: Incorporate sustainability metrics into the objective function, and conduct risk assessments before scaling up.

9. Practical Workflow Example Incorporating AI Optimization

1. Define Objective: Maximize the photoluminescence quantum yield (PLQY) of a CsPbBr₃ perovskite nanocrystal while minimizing lead content. 2. Identify Variables: Precursor concentration, antisolvent type, reaction temperature, and ligand ratio. 3. Collect Initial Data: Perform a fractional factorial design (e.G., 2⁴⁻¹) To generate a baseline dataset of 8 experiments. Measure PLQY, particle size (by DLS), and lead leaching (by ICP-MS). 4. Build Surrogate Model: Train a Gaussian process regressor using the experimental data, including uncertainties from measurement error. 5. Run Bayesian Optimization: Use the surrogate model to propose the next set of synthesis conditions that maximize an acquisition function balancing expected PLQY improvement and lead reduction. 6. Execute Experiments: Automate the reaction using a liquid-handling robot; capture in-line UV-Vis absorption spectra for real-time PLQY estimation. 7. Update Model: Incorporate the new data point, retrain the surrogate, and repeat steps 5-7 until convergence criteria are met (e.G., PLQY > 80% with lead content Validate and Scale-up: Transfer the optimized recipe to a continuous flow reactor; monitor temperature and residence time with PAT tools. Use the same AI framework to fine-tune flow parameters for consistent product quality. 9. Document and Archive: Store all experimental metadata, model versions, and performance metrics in a centralized database for future reproducibility and knowledge transfer.

10. Emerging Terminology at the Intersection of Materials Synthesis and AI

Self-Supervised Learning – A training paradigm where the model learns representations from unlabeled data by solving proxy tasks (e.G., Predicting masked portions of a spectroscopy signal). Enables exploitation of large, unannotated datasets collected during routine synthesis monitoring.

Digital Twin – A virtual replica of a physical synthesis setup that runs in parallel, allowing real-time simulation of process changes and rapid testing of AI-generated recipes before actual execution.

Meta-Learning – “Learning to learn” approaches where the AI system adapts quickly to new synthesis tasks (e.G., A different material system) using knowledge accumulated from prior tasks. Reduces the number of experiments needed for each new material class.

Physics-Informed Neural Networks (PINNs) – Neural networks that embed governing equations (e.G., Mass balance, heat transfer) directly into the loss function, ensuring that predictions respect fundamental physical laws.

Multi-Fidelity Modeling – Combining data of varying accuracy and cost (e.G., Cheap coarse-grained simulations with expensive ab-initio calculations) to build comprehensive predictive models.

Explainable Synthesis Planner – An AI tool that not only suggests synthesis routes but also provides human-readable rationales (e.G., “High temperature promotes phase X formation due to reduced Gibbs free energy”) to foster trust and adoption.

Hybrid Experimental-Computational Loop – An integrated workflow where experimental results feed into computational models (e.G., DFT calculations of formation energies), and the refined computational insights guide the next set of experiments, creating a closed-loop discovery engine.

Quantum-Inspired Optimization – Algorithms that mimic quantum annealing or other quantum phenomena to explore vast synthesis parameter spaces more efficiently than classical heuristics.

Data-Centric Engineering – A shift from model-centric approaches to emphasizing the quality, provenance, and governance of data collected during synthesis, recognizing that reliable AI outcomes depend fundamentally on trustworthy data.

Responsible AI for Materials – Frameworks that incorporate ethical considerations, bias detection, and transparency in AI-driven materials design, ensuring that new materials do not inadvertently exacerbate environmental or societal issues.

These terms, definitions, and contextual examples provide a comprehensive vocabulary foundation for students and practitioners engaged in advanced materials synthesis, especially when leveraging AI for optimization. Mastery of this lexicon enables clear articulation of experimental plans, effective interpretation of literature, and seamless collaboration with data scientists and engineers developing the next generation of high-performance, sustainably produced materials.