Building a Decision-Driven Materials Discovery Institute: Early Insights from MDRI

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1. Introduction

Globally, materials discovery is undergoing a structural shift driven by urgent needs in energy transition, manufacturing resilience, safety, and sustainability, with the United States playing a central role through increased federal investment and institutional innovation. While these investments have rapidly expanded laboratory automation, high-throughput experimentation, and artificial intelligence (AI), many discovery efforts still struggle to convert experimental speed into timely, trustworthy decisions. Fragmented analytics, inconsistent metadata, and delayed integration of real-world constraints continue to slow translation and increase risk—often producing faster experiments without faster learning or clearer pathways to deployment.

As a nonprofit research organization grounded in safety science and public trust, UL Research Institutes operates at the interface of academia, industry, and government. Within UL Research Institutes, the Materials Discovery Research Institute (MDRI) was launched in September 2024 to establish a modern, decision-driven model for accelerated materials discovery that explicitly connects early-stage research with downstream deployment. MDRI is designed to reduce friction between discovery and implementation by coupling digital-first research practices with application-informed evaluation and by embedding safety and sustainability considerations early, when they can meaningfully shape which materials and pathways are pursued.

2. Approach and contribution

MDRI is structured around integrated automation frameworks that link synthesis, characterization, analytics, and engineering into a continuous, decision-driven workflow. Automated platforms generate systematic libraries of materials with consistent execution and complete experimental context capture, forming a comparable and traceable foundation for accelerated learning. Standardized, high-throughput characterization enables direct comparison across datasets, while analytics translate raw experimental outputs into decision-ready summaries that support rapid benchmarking, prioritization, and iterative refinement. These summaries are designed to be actionable, emphasizing standardized descriptors, consistency and quality indicators, and comparative baselines that enable fast down-selection across large libraries without waiting for manual interpretation. AI functions primarily as an enabling layer—enhancing comparability, ranking, and navigation across large compositional and process design spaces—rather than operating as a standalone modeling exercise. Safety, sustainability, and manufacturability constraints are embedded early in the workflow to reduce downstream risk and to ensure that acceleration remains aligned with deployability.

In parallel with discovery automation, MDRI is building dedicated engineering capabilities to translate promising materials into functional systems and prototypes. This integration enables early validation under application-relevant conditions, establishes feedback loops from prototype performance back to discovery priorities, and supports advancement toward higher technology readiness levels. MDRI's model emphasizes that translation is not a downstream handoff, but a co-evolving process in which discovery objectives, test environments, and prototype constraints inform one another from the start. This presentation will introduce MDRI's organizational model, digital–physical infrastructure, and initial findings from its first year of operation, including examples of the institute's internally developed tools and workflows that accelerate iteration and improve decision quality. Case examples will include accelerated discovery efforts in electrocatalysts for clean energy applications and advanced adsorbents for environmental remediation and water harvesting. For electrocatalysts, we will highlight how systematic library generation and rapid screening can be paired with decision-ready analytics to accelerate down-selection while maintaining attention to durability-relevant and scale-informed considerations. For adsorbents, we will highlight how structured synthesis–characterization–analysis loops enable faster mapping of structure–property relationships and application-context constraints. Across both domains, emphasis will be placed on how integrated analytics, engineering translation, and decision-driven workflows are shortening iteration cycles and advancing promising materials toward functional prototypes and higher technology readiness levels, including TRL 7. Together, these early results illustrate how a safety-informed, institutionally grounded discovery model can convert automation and AI investments into faster, more reliable pathways from materials innovation to real-world impact across sectors of national importance.