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Self-driving laboratories in Korea: a new era of autonomous discovery

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Self-driving laboratories (SDLs) integrate automation, robotics, and artificial intelligence to accelerate discovery through closed-loop experimentation. Korea offers a particularly strong foundation for SDL adoption, supported by globally competitive industries in semiconductors, batteries, and chemical manufacturing. This Perspective highlights SDL initiatives across Korean academia and industry. In nanomaterials and catalysis, robotic coin-cell assembly, autonomous nanoparticle synthesis, and automated solid oxide cell workflows are advancing reproducibility and throughput. In organic chemistry and bioengineering, AI-driven robotic chemists, ultrafast flow platforms, and autonomous nanoparticle manufacturing exemplify rapid data-driven optimization. National-scale initiatives, including the K-Biofoundry, extend SDL principles to synthetic biology. Together, these efforts position Korea as a global testbed for SDLs, linking discovery to production.

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1. Introduction

Self-driving laboratories (SDLs) have emerged as a transformative paradigm in scientific research, integrating laboratory automation, robotics, and artificial intelligence (AI) to establish closed-loop experimentation.[1–7] While traditional laboratory automation systems primarily addressed repetitive manual tasks, SDLs go beyond mere automation by incorporating machine learning algorithms that interpret results and propose new conditions, thereby combining human creativity with computational power. This integration accelerates the discovery-to-production cycle and enhances reproducibility, scalability, and safety. From a broader socio-economic perspective, SDLs also address a pressing structural challenge: the increasing scarcity of skilled researchers caused by demographic trends such as aging populations and declining birth rates.[8,9] By reducing reliance on labor-intensive manual experimentation, SDLs provide a path to sustain scientific productivity under limited human resources.

Korea presents a particularly compelling environment for SDL adoption. The nation has cultivated world-leading industries in semiconductors, batteries, and chemical manufacturing, and has accumulated decades of expertise in process automation and precision engineering. This industrial foundation creates fertile ground for extending automation principles from the factory floor into the research laboratory. Historically, Korea was an early adopter of modular laboratory automation: in 1994, Samsung Medical Center introduced a total laboratory automation (TLA) system that integrated biochemical and immunoassay analyzers through a conveyor-based modular platform.[10] This early implementation highlights Korea's longstanding emphasis on integration and modularity, principles that resonate strongly with the SDL vision.

Governmental and industrial strategies are accelerating this trajectory. According to the 2023 National Robot Industry Survey, demand for manufacturing and professional service

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robots is increasing at an annual average rate of 1.4%, and multiple seed-type R&D programs are being initiated across sectors.[11] In October 2024, the Ministry of Trade, Industry, and Energy announced the "AI + R&D Strategy" and "Industrial Data Utilization Roadmap", targeting the introduction of 500 autonomous laboratories by 2030.[12] Market forecasts predict the Korean laboratory automation sector will grow from USD 125.8 million in 2024 to over USD 320 million by 2035, reflecting a compound annual growth rate of 7.46%.[13]

In this context, this perspective provides an overview of SDL research and implementation in Korea. To distinguish domain-specific applications from cross-cutting implementation layers, Sections 2–4 focus on representative Korean SDL examples in nanomaterials and catalysis, organic and inorganic synthesis, and bioengineering. Section 5 then consolidates broadly applicable SDL capabilities, including orchestration, robotic execution, active-learning-based planning, safety monitoring, and interoperability/standardization. Section 6 discusses industrial adoption, Section 7 outlines future opportunities and remaining challenges for building a sustainable SDL ecosystem in Korea, and Section 8 concludes with perspectives on Korea's potential contributions to global autonomous experimentation.

2. SDLs for nanomaterials and catalysis

This section focuses on application-side progress in Korean SDLs for nanomaterials and catalysis, while cross-cutting methodological and systems-level capabilities are discussed later in Section 5. The examples below illustrate how autonomous experimentation is being applied to battery materials, nanoparticle synthesis, and high-throughput catalyst workflows, with an emphasis on representative Korean platforms and use cases.

2.1. Battery materials

The global expansion of electric vehicles and the tightening of carbon regulations have intensified the need for advanced secondary batteries.[14] Although lithium-ion batteries dominate the market, their safety concerns—particularly flammability and explosion risks—have driven research into flame-retardant liquid electrolytes and solid-state ceramic electrolytes.[15,16] At the same time, achieving higher energy density at reduced cost has emerged as a critical requirement, motivating the development of next-generation cathode materials. However, these material systems are characterized by vast compositional spaces and strong sensitivity to subtle changes in composition and processing, which makes outcomes highly dependent on precise control of materials handling and synthesis conditions. As a result, conventional trial-and-error or expert intuition-guided experimentation is often constrained by limited throughput and reproducibility, motivating SDL approaches that integrate automation and data-driven analysis for systematic exploration.

To address these limitations in liquid electrolyte research, efforts in Korea have aimed to automate electrolyte formulation, cell fabrication, and performance testing through an integrated platform termed ALBATROSS (Automated Laboratory for Battery Testing, Optimization, and Research of Secondary Systems), as shown in Fig. 1a.[17] By standardizing assembly procedures and testing protocols, ALBATROSS improves reproducibility while substantially increasing experimental throughput compared to conventional manual workflows. The platform enables systematic acquisition of charge–discharge cycling and electrochemical impedance spectroscopy (EIS) data across diverse operating conditions, with a relative standard deviation in discharge capacity typically within ~1%, comparable to that achieved by experienced researchers.

To ensure high data reliability, ALBATROSS is installed within an argon-filled glovebox (Fig. 1b), where moisture and oxygen levels are controlled below the ppm level to minimize environmental variability during electrolyte handling and cell assembly.[17] The system is capable of autonomously assembling and initiating tests for up to 48 coin cells without human

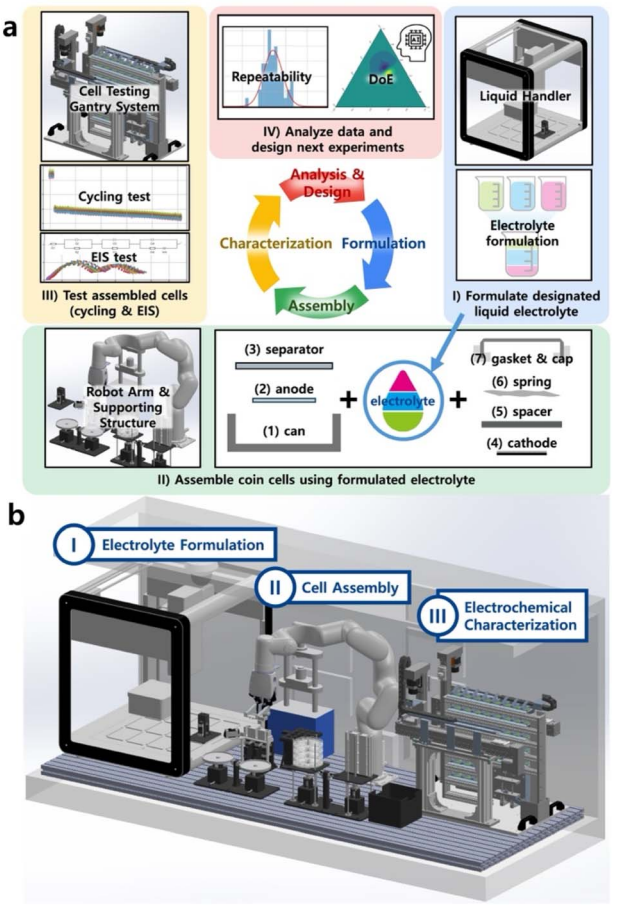

Fig. 1 ALBATROSS platform for automated liquid electrolyte formulation, coin-cell assembly, and electrochemical characterization. (a) Closed-loop workflow integrating electrolyte formulation, robotic cell assembly, cycling and EIS measurements, and data-driven experimental design. (b) Three-dimensional rendering of the ALBATROSS system installed inside an Ar-filled glovebox. AI-driven decision-making can enter the loop at the data-driven experimental design step, where cycling/EIS results are analyzed to propose the next electrolyte formulation. Reproduced from ref. 17 with permission from the authors.

intervention. While the assembly time per cell, on the order of a few minutes, is comparable to that of skilled experimentalists, the key advantage lies in the platform's ability to operate continuously, enabling uninterrupted fabrication and evaluation of large cell batches. By coupling standardized assembly conditions and controlled glovebox environment metadata with cycling/EIS outputs, ALBATROSS supports the creation of reproducible, machine-actionable electrochemical datasets for downstream analysis and model-assisted optimization.

Solid electrolytes and cathode materials share a largely common experimental workflow, encompassing precursor handling, weighing, mixing, pelletizing, thermal processing, and structural characterization by X-ray diffraction. This process-level overlap makes them particularly suitable for unified SDL frameworks, where automation and data-driven feedback can be applied across multiple materials classes. However, in closed-loop experimentation, solid-state synthesis remains a dominant bottleneck. Conventional solid-state reactions typically require more than 10 hours of high-temperature processing per composition, severely limiting iteration speed and rendering systematic exploration impractical even with automated handling and characterization. To address the time-intensive nature of conventional solid-state synthesis, previous studies have proposed ultrafast high-temperature synthesis (UHS) as a rapid alternative that significantly shortens reaction and densification times. The feasibility of UHS was first demonstrated in manual experiments, where garnet-type solid electrolytes were synthesized within minutes while retaining phase purity and ionic conductivity comparable to those obtained *via* conventional routes.

Building on this concept, recent efforts in Korea have begun to investigate UHS as a strategy to replace the principal bottleneck in closed-loop experimentation for solid-state battery materials, with emerging SDL-oriented platforms targeting solid electrolytes and next-generation cathode materials.[18,19] Collaborative efforts with Merck KGaA have explored UHS to accelerate sodium solid electrolyte discovery within automated and data-driven workflows,[18] while a separate SDL initiative with POSCO Holdings focuses on disordered rock-salt Li-excess (DRX) cathode materials.[19] In the latter case, DRX cathode materials can be synthesized *via* UHS within approximately 20 minutes and exhibit particle size, crystal structure, and electrochemical performance comparable to those of materials prepared using conventional solid-state methods, supporting UHS for rapid screening and early identification of promising compositions.[20] By replacing the most time-consuming synthesis step with UHS, these SDL efforts substantially accelerate iteration cycles for complex battery materials spaces.

2.2. Nanoparticle synthesis

Nanoparticles (NPs) are widely applied in solar cells, catalysis, chemical sensing, and biomedical systems due to their tunable optical and electronic properties.[21–24] However, their synthesis is highly sensitive to many parameters, including precursor concentration, injection rate, solution volume, aging time, and reaction sequence. Conventional combinatorial approaches such as grid exploration are impractical due to the combinatorial explosion of possible conditions. To overcome this challenge, an autonomous nanoparticle synthesis platform was developed in Korea that integrates (i) a batch synthesis module, (ii) a UV-vis spectroscopy module, and (iii) a Bayesian optimization AI module, all interconnected through a robotic arm to form a closed-loop system (Fig. 2a and b).[25] The batch synthesis module incorporates a custom vial storage system that distinguishes used and unused vials, a stirring machine, a stock solution system, syringe pumps, dispensers, and an XYZ actuator-based solution dispensing unit. Following synthesis, nanoparticles are automatically transferred to the UV-vis module for optical characterization. The resulting spectra are fed into a Bayesian optimizer (based on algorithms first demonstrated for mobile robotic chemistry), which proposes the next experimental conditions.[26]

The primary goal was to synthesize Ag nanoparticles with user-defined absorption spectra, relevant to applications in

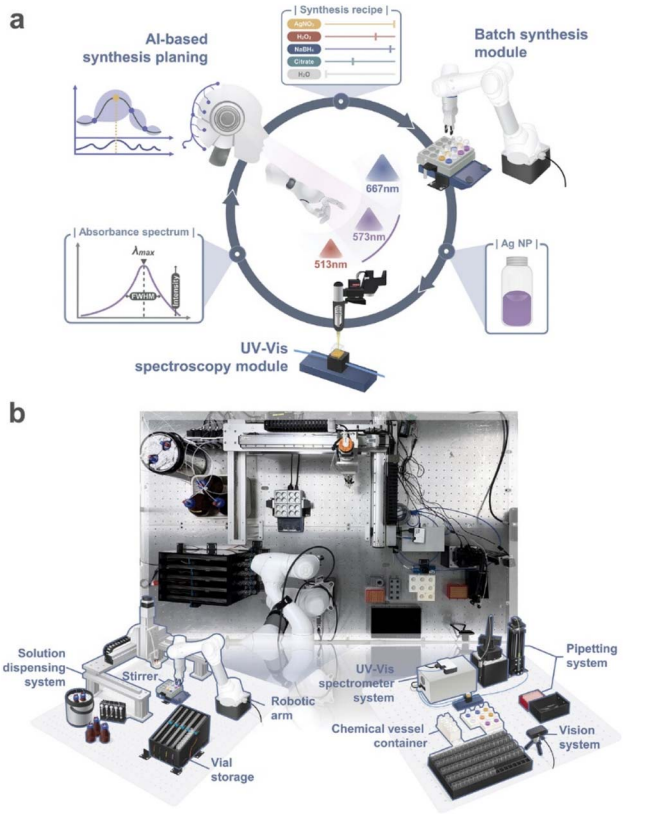

Fig. 2 The autonomous laboratory platform for bespoke NP design with target optical properties. (a) Scheme of the closed-loop operations for the development of Ag NPs with desired absorption spectra, as exemplified by λ_{max} of 513, 573, and 667 nm. (b) A bird's eye view image of our autonomous laboratory and schematic illustrations of the batch NP synthesis module (left) and UV-vis spectroscopy module (right). The synthesis module automatically synthesizes colloidal Ag NPs, while the UV-vis spectroscopy module extracts the optical properties of the synthesized NPs. AI-driven decision-making enters the loop when the Bayesian optimizer proposes the next synthesis conditions based on measured UV-vis spectra. Reproduced from ref. 25 with permission from Wiley-VCH GmbH, licensed under CC BY, copyright 2024.

biomedical imaging, sensors, light-emitting diodes, and solar cell sensitizers. While commercial nanoparticles with specific light-trapping properties exist, their recipes are often proprietary, limiting reproducibility. Using only five reagents ($AgNO_3$, H_2O_2, $NaBH_4$, citrate, and H_2O) at room temperature, the autonomous platform optimized reagent volumes to achieve targeted optical properties.

Remarkably, the system achieved desired absorption peaks within 200 iterations, whereas brute-force grid exploration would require on the order of 10^9 experiments. The platform also demonstrated flexibility by varying the importance weights of spectral parameters (wavelength, FWHM, peak intensity) while maintaining convergence. Beyond optimization, SHapley Additive exPlanations (SHAP)[25] analysis was applied to interpret the role of each reagent, revealing that $AgNO_3$ and H_2O_2 strongly influence λ_{max}, whereas citrate significantly affects FWHM and peak intensity. These results suggest that autonomous platforms can yield mechanistic insight by systematically interrogating parameter sensitivities. Each closed-loop iteration produces a structured record linking reagent volumes and process settings to UV-vis spectra, enabling both optimization reproducibility and reuse for model training and sensitivity analysis.

2.3. High-throughput evolution of nanomaterials

In parallel, autonomous workflows for catalyst synthesis are being developed in Korea, including ongoing efforts at the Chemical Data-Driven Research Center, Korea Research Institute of Chemical Technology. The system targets reproducible synthesis of metal-supported catalysts *via* impregnation-based workflows using solid powders and liquid precursors. It is modularized into supply, mixing, and drying units, which are coordinated by a robotic arm to execute catalyst synthesis recipes autonomously (Fig. 3). Unlike conventional human-operated experiments that proceed sequentially, the robotic system supports parallel synthesis across multiple modules, thereby increasing throughput. This modular architecture is material-agnostic and can be extended beyond catalyst synthesis to a broad range of nanomaterials.

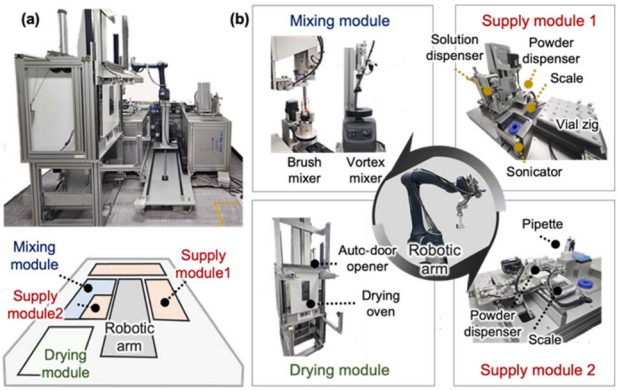

Fig. 3 (a) Schematic view of an automated laboratory for catalyst synthesis and (b) its modules orchestrated by a robotic arm.

During the supply stage, solid powders are dispensed using automated mass-controlled dispensers, while liquid precursors are aliquoted *via* pipetting systems. The mixing module integrates multiple mixing devices—including brush mixers, sonicators, and vortex mixers—to enable flexible combinations of mixing modes tailored to specific material systems. Rapid prototyping based on 3D printing is used to accelerate design–test–feedback cycles for mixing hardware. All modules are coordinated through a programmable-logic controller (PLC), which synchronizes robotic arm motion, equipment operation, recipe execution, and data logging. Data acquisition and post-processing are handled through Python-based pipelines.

3. SDLs for organic and inorganic synthesis

This section presents domain-specific SDL examples in organic and inorganic synthesis. Although the studies discussed here are rooted in chemistry applications, several of the enabling principles—such as robotic execution, experiment planning, and workflow coordination—extend across domains and are therefore consolidated later in Section 5.

3.1. Autonomous organic synthesis

Organic molecules play central roles in diverse domains, ranging from polymers and solvents to catalysts and pharmaceuticals.[27,28] Yet the design of autonomous systems for organic synthesis remains particularly challenging, owing to the vast combinatorial space of possible reaction conditions and the intrinsic complexity of multi-step synthetic pathways.

To effectively explore organic chemistry, an autonomous laboratory termed Synbot was established for single-step organic synthesis.[29] The Synbot platform distinguishes itself by a clear division between AI software and robotic software layers. The AI module modifies reaction recipes (RCPs), analyzes outcome data, and proposes the next input parameters, while the robotic layer executes precursor dispensing, reactor operation, and analysis. The workflow proceeds as follows: (1) precursors are dispensed into vials and automatically transferred into designated reactors; (2) six independent reactors enable reactions under variable temperatures; (3) reaction progress is monitored in real time using LC-MS.

This closed-loop cycle allows the system to assess synthesis state and determine whether to continue, modify, or terminate a pathway. Synbot can accumulate structured reaction records that connect recipe variants and reactor conditions to LC-MS outcomes, providing a foundation for reusable datasets in autonomous reaction optimization. While the platform is still in the database accumulation phase, the expectation is that as the dataset grows, the AI module will achieve increasingly reliable predictions and higher probabilities of converging on optimal conditions.

3.2. Robot-assisted reaction hyperspace mapping

Reaction hyperspace mapping is broadly relevant as a general SDL strategy for systematic reaction-space exploration and

dataset generation. To explore large and complex reaction spaces in an unbiased, systematic manner, a robot-assisted experimental platform has been proposed for mapping organic reaction hyperspaces.[30] Rather than optimizing a single target reaction, the system performs thousands of microscale experiments across wide ranges of reagent ratios, solvents, and temperatures to construct a quantitative representation of chemical reactivity. Reaction mixtures are analyzed in real time using UV-vis spectroscopy, and acquired spectra are processed through spectral unmixing algorithms to determine product distributions with minimal error.

From these high-dimensional datasets, the platform reconstructs reaction networks that reveal mechanistic connections, switching behaviors, and hidden intermediates across classical transformations such as SN1, E1, Ugi, and Hantzsch reactions. This study demonstrates how robotic automation and data-driven analysis can transform empirical screening into systematic exploration. Within the SDL context, such "reactivity mapping" provides a general strategy for discovering transformations and understanding complex reaction dynamics.

3.3. Organic synthesis prediction

Predicting outcomes of organic reactions remains one of the most intellectually demanding challenges in chemistry. Accurate prediction is crucial for rational molecular design, new materials discovery, and drug development, yet even expert chemists often struggle to generalize across diverse reaction classes. To address these limitations, several machine learning models for predicting molecular reactions have been proposed.[31–33] Notably, in Korea, a chemistry-motivated graph neural network model, LocalTransform, was proposed to predict organic reactivity using a generalized reaction representation.[34] The core innovation lies in the Generalized Reaction Template (GRT), which eliminates explicit atom-type and functional-group labels and instead encodes local atomic configuration changes derived from atom mapping between reactants and products. By learning transferable local transformations, LocalTransform improves coverage and scalability relative to earlier template-based methods. A library of only ~3000 GRTs was sufficient to describe 99.7% of all test reactions, indicating strong generalization.

In the inference phase, LocalTransform identifies the applicable GRT at the predicted reaction center and applies it to generate probable product structures. Benchmarking on USPTO-480 k showed that LocalTransform outperformed widely used sequence-based models such as Molecular Transformer[31] and Augmented Transformer[33] in top-1 accuracy. Related models have also been developed in Korea for retrosynthesis, precise reaction description, and synthetic accessibility prediction.[35–37]

A key bottleneck, however, is that most training corpora describe only reactants and final products, limiting interpretability. To address this, a two-step framework, MechFinder, was developed to generate mechanistic annotations by combining automatically extracted reaction templates with expert-curated mechanistic templates that encode electron-flow logic.[38] This produced mech-USPTO-31 K (31 364 reactions) with explicit pathways, intermediates, and electron – movement diagrams. Such mechanism-aware data can enable next-generation models that predict not only products but also intermediates and trajectories, improving interpretability and robustness.

Together, these studies illustrate how chemistry-grounded AI models can complement SDL frameworks by guiding experiment design, screening, and hypothesis generation with near-human predictive capability.

3.4. Inorganic synthesis

Efforts have also been made to predict synthesizability and synthesis methods of inorganic materials to reduce trial-and-error and accelerate materials discovery within SDLs.[39–41] These studies aim to bridge computational materials design and experimental realization by learning patterns that govern whether a compound can be synthesized and how it can be made.

In Korea, a data-driven model for inorganic synthesizability prediction has been proposed using a structure-based partially supervised learning framework with positive – unlabeled (PU) learning and graph convolutional neural networks (Fig. 4a).[42] The resulting crystal-likeness score (CLscore) quantifies the likelihood that a given crystal structure is experimentally synthesizable, achieving over 87% accuracy for known materials. Subsequent frameworks have incorporated transfer learning and fine-tuned large language models (LLMs).[43–46] More recently, redesign processes have been proposed to convert previously unsynthesizable structures into synthesizable ones, expanding viable candidate pools.[47]

Beyond feasibility assessment, a retrosynthetic model for predicting synthesis methods has also been developed.[48] ElemwiseRetro predicts solid-state synthesis recipes, including precursor combinations and reaction temperatures, using an element-wise, template-based graph neural network (Fig. 4b). The model achieved 78.6% top-1 and 96.1% top-5 accuracy, and confidence scores correlated positively with prediction accuracy—useful for prioritizing synthesis attempts in SDL workflows.[49] A further developed retrieval-based model (Retrieval-Retro) has also been suggested in Korea.[50]

Together, these advances enable models that not only assess the synthesizability of materials but also propose concrete experimental routes, paving the way toward autonomous inorganic synthesis in self-driving laboratories.

3.5. Ultrafast flow chemistry

The demand for rapid and cost-effective drug development has underscored the importance of ultrafast flow chemistry. Conventional batch synthesis often struggles to control unstable intermediates and highly reactive reagents, which hinder the exploration of new reaction pathways.

In Korea, an automated microreactor platform (AMP) integrating robotic operation, data collection, and inline FT-IR was developed to realize continuous, self-optimizing ultrafast flow chemistry (Fig. 5).[51] The AMP comprises syringe pumps, solenoid valves, a circulating thermostat with a cooling chamber,

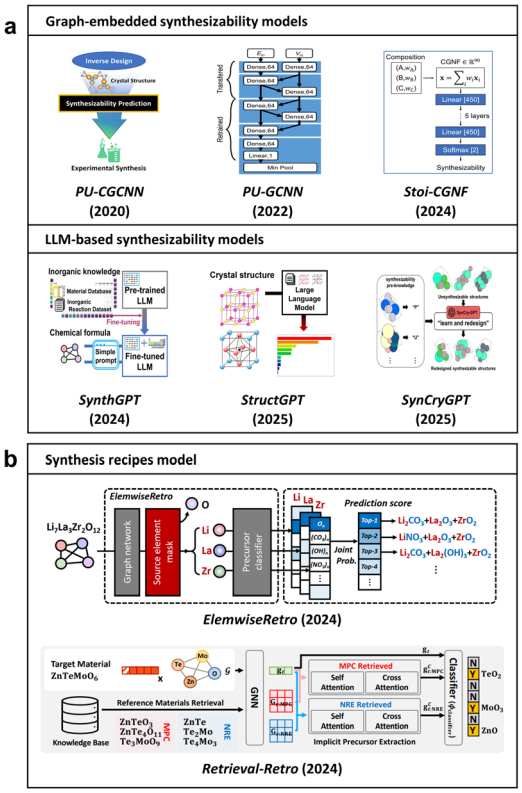

Fig. 4 Overview of representative inorganic synthesis predictive models derived from accumulated synthesis data. Various synthesizability prediction frameworks, including graph-embedded neural network models and large language model (LLM)-based architectures.

pressure sensors, and analytical devices, all orchestrated by a central computer. Key parameters such as mixing efficiency, residence time, and reaction temperature are systematically varied, while Bayesian optimization (BO) refines the search for optimal conditions.

The system was validated in a user-planning mode (testing predefined ranges across 80 conditions) and subsequently in an AI-planning mode, where a Gaussian process – based expected improvement algorithm autonomously selected experimental conditions. The system identified optimal yield conditions within 10 iterations. Furthermore, the AMP generated an *S*-benzylic thioquinazolinone library, producing nine products within 20 minutes.[51] These results show how SDL-enabled ultrafast flow chemistry can reduce synthesis times from hours per day to minutes while maintaining accuracy and efficiency even for unstable intermediates. The AMP generates iteration-indexed datasets linking flow parameters and temperature to inline FT-IR signals and yields, which can be reused for benchmarking and data-driven condition optimization.

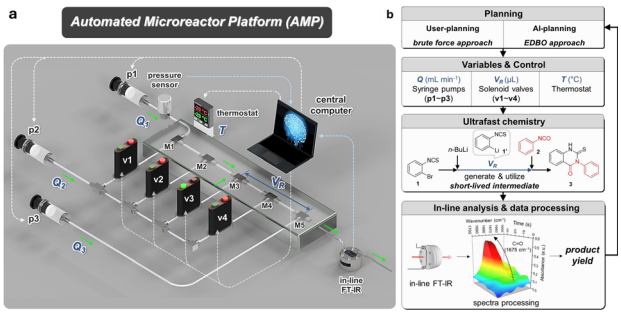

Fig. 5 Automated microreactor platform (AMP) for efficient screening and optimization of ultrafast chemistry. (a) Schematic diagram of the AMP showing automatic control of three variables (flow rate Q, reaction volume V_R, and temperature T) and real-time. AI-driven decision-making enters the loop when BO selects the next flow conditions based on inline measurements. Reproduced from ref. 51 with permission from Elsevier, Copyright 2023.

4. SDLs for bioengineering

Compared with the chemistry-focused examples in Section 3, the SDL efforts discussed in this section are centered on bioengineering and biomanufacturing workflows, particularly those involving drug-delivering nanoparticle formulation, purification, and infrastructure for design–build–test–learn (DBTL) cycles.

4.1. Autonomous nanoparticle manufacturing for drug delivery

In drug delivery systems (DDS), SDL principles have been applied through development of an autonomous, integrated microfluidic (AIM) platform.[49] The AIM platform comprises a synthesis module and a purification module, seamlessly coupled with inline analysis.

In the system, the Automated Nanoparticle Synthesizer (ANS) enables nanoparticle fabrication *via* nanoprecipitation with precise control of particle size and drug loading efficiency. Using this platform, doxorubicin-loaded liposomes and polymer nanoparticles were synthesized reproducibly at target size and concentration. A multi-objective Bayesian optimization (MOBO) algorithm autonomously tuned nanoparticle properties and drug-loading parameters (Fig. 6).[49] Extended operation demonstrated high reproducibility with negligible drift over cycles, and synthesis times were reduced from days to less than 20 minutes.

The purification module, termed the Multi-Buffer Injector (MBI), employs ultrafast flow dialysis to remove impurities and unencapsulated drugs while performing inline characterization. Encapsulated doxorubicin (DOX) can be released by methanol-induced nanoparticle disruption and quantified *via* UV-vis spectroscopy, allowing determination of encapsulation efficiency (EE) and expected loading capacity (ELC). Performance evaluation confirmed stability across multiple cycles, with >15 purification runs maintaining target removal efficiency.[49] The AIM platform captures synthesis and purification settings alongside particle metrics and drug-loading readouts (*e.g.*, EE and ELC), enabling structured datasets suitable for reproducible formulation development (Fig. 7).

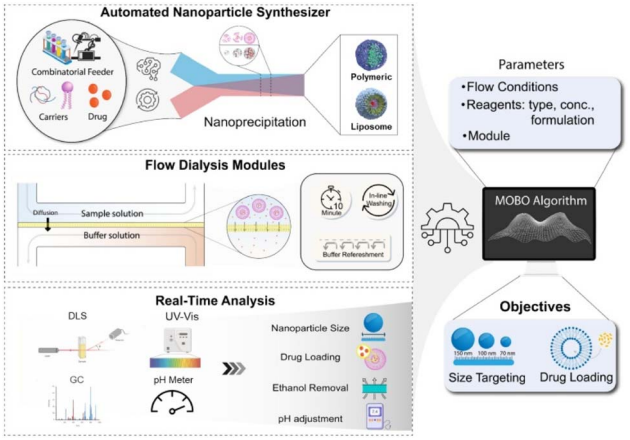

Fig. 6 Schematic illustration of the autonomous, integrated, microfluidic (AIM) platform. Automated Nanoparticle Synthesizer (ANS) platform for autonomous synthesis of liposomes. AI-driven decision-making enters the loop when MOBO proposes the next synthesis parameters based on measured objectives. Reproduced from ref. 49 with permission from Elsevier, Copyright 2024.

4.2. National biofoundry initiatives as infrastructure-level DBTL capability

This subsection is included not as a single biological application example, but as an infrastructure-level SDL capability that supports design–build–test–learn (DBTL) workflows at institutional scale. Beyond individual laboratories, Korea has also invested in institutional-scale SDL initiatives. The K-Biofoundry, jointly operated by the Korea Research Institute of Bioscience and Biotechnology (KRIBB) and KAIST, exemplifies national commitment to integrating SDL principles into synthetic biology. The biofoundry accelerates the design–build–test–learn (DBTL) cycle by employing robotics for strain construction and AI/ML algorithms for high-throughput data analysis.

Biological research is typically constrained by time-intensive cultivation steps and the need to process large combinatorial datasets for DNA sequence design and evaluation. By delegating repetitive culturing and screening tasks to robots and leveraging AI for sequence assembly and functional analysis, the K-Biofoundry aims to improve throughput and efficiency. As an infrastructure-level initiative, it also provides a pathway toward more standardized workflows and structured data generation for broader community reuse.

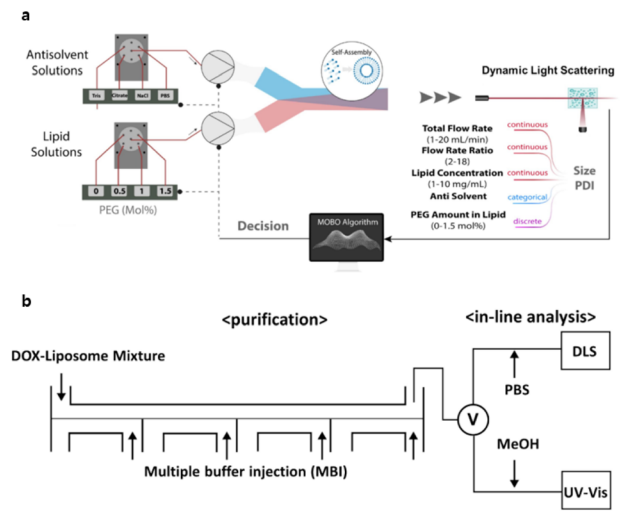

Fig. 7 Simplified diagram of automated synthesizer, purification and in-line analysis system. (a) Overall schematic diagram for ANS module. Reprinted from ref. 45 with permission from Elsevier, Copyright 2024. (b) Purification schematic diagram of continuous-flow MBI module, coupled with in-line analysis. Reprinted from ref. 49 with permission from Elsevier, Copyright 2024.

5. Software and orchestration systems

The SDL examples discussed in Sections 2–4 highlight application-specific progress in Korea, but many of the enabling concepts underlying these platforms are shared across domains. These include orchestration, robotic execution, active-learning-based experiment planning, safety monitoring, and interoperability of data and workflows. To avoid repeating these methodological elements within each domain section, they are discussed together here as cross-cutting capabilities for scalable SDL implementation.

5.1. OCTOPUS OS

A central challenge in SDL implementation lies in orchestrating multiple experimental modules into a seamless and efficient workflow. To address this, OCTOPUS (operation control system for task optimization and job parallelization *via* a user-optimal scheduler) enables task optimization and parallelization under a user-optimal scheduler (Fig. 8).[52] OCTOPUS adopts a hierarchical architecture comprising three nodes: interface nodes, master nodes, and module nodes.

The interface node manages client logins, enforces security protocols, and handles user commands. To ensure broad accessibility, the system employs standardized TCP/IP protocols compatible with multiple programming languages, while UDP-based notifications enable real-time alerts and emergency shutdowns. The master node orchestrates experiments by scheduling tasks, parallelizing jobs, and allocating resources. Through job parallelization, OCTOPUS reduces total runtime across multi-user requests. Conflict resolution is achieved *via* masking tables that prevent overlapping use of shared hardware (*e.g.*, robotic arms).[52] The module node supervises individual experimental units. SDLs under OCTOPUS are organized hierarchically: the top-level platform, subdivided into modules, further into tasks, and ultimately into actions.

To facilitate rapid expansion, the team also developed a GPT-based Copilot that auto-generates code for integrating new modules. By applying few-shot prompt engineering, Copilot reduces manual coding effort, enabling new hardware modules to be incorporated with minimal technical barriers.[52] Beyond execution, JSON-based job scripts and action/event traces provide run-level provenance that supports reproducibility, failure filtering, and downstream curation for dataset reuse across sites.

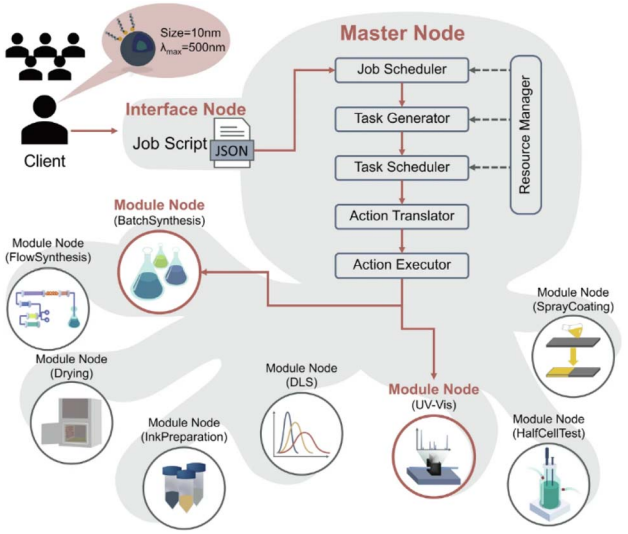

Fig. 8 The architecture of OCTOPUS comprises three main components, the interface node, master node, and module nodes. Multiple clients submit job scripts *via* CLI based on the JavaScript object notation (JSON) format. The master node manages the submitted. Reproduced from ref. 52 with permission from Springer Nature, Copyright 2024.

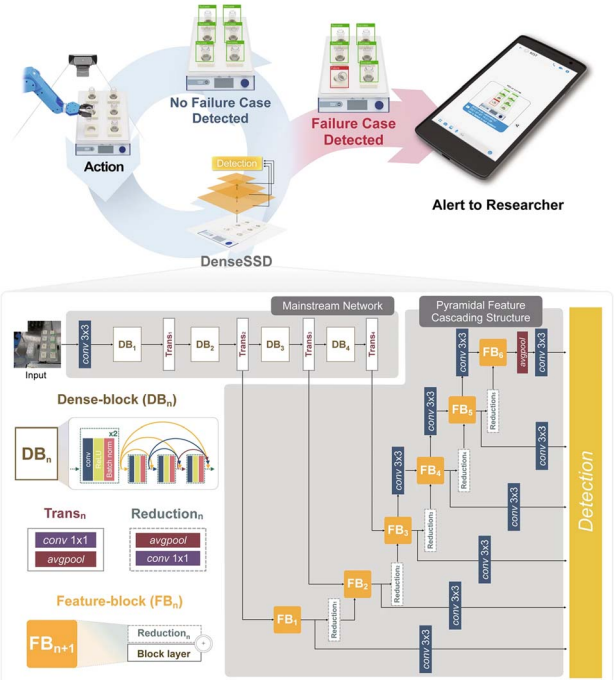

Fig. 9 Workflow of the vial positioning detection system based on DenseSSD. An action is defined as the movement of the robot arm to relocate each vial to its holder. Green and red boxes represent the predicted bounding boxes for the success and failure. Reproduced from ref. 53 with permission from Springer Nature, licensed under CC BY, copyright 2024.

5.2. Vision-based risk detection

Minimizing human intervention in SDLs heightens the importance of automated risk detection and safety monitoring. Conventional approaches relying on robotic pressure sensors are limited when handling hazardous reagents, particularly with transparent or semi-transparent vessels.

To address this, DenseSSD, a deep-learning – based vision system optimized for laboratory environments, was introduced to enhance automated visual recognition in SDLs (Fig. 9).[52] DenseSSD consists of a mainstream network and a pyramidal feature cascading structure for multi-scale feature extraction. Training employed extensive data augmentation to improve robustness. The model distinguishes successful vial placements from failure cases (*e.g.*, fall-out, lie-down, lean-in, stand-on).[53]

With >95% detection precision, DenseSSD outperformed conventional detectors in classifying transparent and semi-transparent vials, regardless of whether they were filled or empty.[53] This vision-based monitoring capability is critical for SDL safety and for protecting data integrity by preventing failed operations from contaminating closed-loop datasets.

5.3. Modular frameworks: ModuFlow

A modular orchestration framework, ModuFlow, is being developed by Seoul National University to standardize SDL operations across heterogeneous instruments. Whereas many existing SDL platforms remain customized for specific laboratories, ModuFlow adopts a modular architecture to enable interoperability and expandability. By treating workflows as combinable modules, ModuFlow facilitates integration of diverse processes (synthesis, coating, measurement) into unified autonomous systems. Together with OCTOPUS[52] and DenseSSD,[53] ModuFlow contributes to foundational software/hardware infrastructure for scalable SDL ecosystems.

5.4. Interoperability and standardization issues

Interoperability remains a key bottleneck for scaling self-driving laboratories (SDLs) beyond single-lab deployments. In practice, failures most often arise at two interfaces: (i) experimental provenance, where execution records and measurement outputs are captured in separate systems without reliable linkage, and (ii) workflow semantics, where identical actions and events carry different operational meaning across platforms. These issues become more consequential as Korean SDL efforts expand across universities, national institutes, and industrial R&D, where conventions for identifiers, metadata, and quality control frequently differ.

A representative provenance challenge appears in battery-oriented SDLs (*e.g.*, glovebox-integrated coin-cell assembly and testing), which produce parallel streams from automation (recipes, dispense volumes, component lots, environment) and instruments (cycler/EIS channel-indexed files, protocols, settings). When sample identifiers do not map cleanly to instrument channel identifiers—or when key context (formation protocol versions, glovebox O_2/H_2O, instrument settings) is stored outside the dataset—reconstructing a machine-actionable run becomes labor-intensive and undermines cross-lab comparison and repository submission. A practical near-term remedy is to enforce a minimal coin-cell run record at

the orchestration layer, capturing persistent run/sample IDs, environment snapshots, recipe/protocol versioning, cycler/channel mapping, and essential instrument settings.

Workflow portability faces a complementary challenge. Orchestration systems such as OCTOPUS translate job scripts into hierarchical tasks/actions and device commands, yet the same action label (*e.g.*, "dispense," "transfer") can imply different priming/washing steps, success criteria, or recovery behaviors across SDL stacks. Safety/quality signals (*e.g.*, vision-detected placement failures) are similarly difficult to reuse unless event/exception logs are standardized. Near-term remedies include a shared action vocabulary with explicit pre-/post-conditions, a harmonized failure-mode and recovery-policy taxonomy, and standardized event/exception logging that downstream planners and curators can interpret consistently.

SDL-specific standardization in Korea is still nascent and project-driven, so coordinated alignment across academia–institutes–industry is increasingly needed—while remaining compatible with emerging global standards. A pragmatic path is a layered strategy: adopt global interface/data practices where mature (*e.g.*, device/service interfaces and common data packaging) and define Korea-specific minimum viable interoperability profiles that can be mapped to national data infrastructure (*e.g.*, K-MDS). Concretely, we suggest prioritizing: (i) workflow-specific minimal run records, (ii) an action/exception schema implementable in orchestration platforms, and (iii) lightweight "crosswalks" from run records and logs to repository-ready fields for benchmarking and reuse.

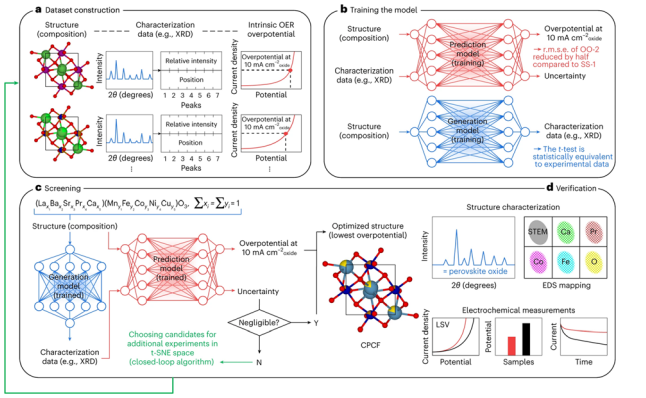

Fig. 10 (a) The initial dataset of 30 four-metal perovskite oxides provides compositional and structural data in graph format, characterization (X-ray diffraction, XRD) data and OER performance data. θ represents the angle between incident beam of the X-ray and a given crystal lattice plane. (b and c), The red (prediction) model and the blue (generation) model are individually trained (b) and combined (c) for the screening process. Additional experiments are carried out if the prediction uncertainty is not negligible. Y, yes; N, no. (d) The predicted optimal oxide is synthesized and undergoes structure characterization and electrochemical performance verification (for example, linear sweep voltammetry, LSV). Reproduced from ref. 56 with permission from Springer Nature, Copyright 2023.

5.5 Active learning for materials discovery

Active learning is not limited to a specific materials domain, but is instead a broadly applicable SDL planning strategy for reducing experimental burden while improving model accuracy. At the intersection of machine learning and autonomous experimentation, active learning has emerged as a crucial strategy to accelerate materials discovery while minimizing the number of required experiments.[54,55] A representative study demonstrated how active learning can guide discovery of high-performance electrocatalysts using only a limited dataset (Fig. 10).[56] Thirty quaternary perovskite oxides were synthesized, and their compositions, XRD patterns, and oxygen evolution reaction (OER) overpotentials were measured to construct an initial dataset. Using these data, the researchers trained a machine learning model correlating structural descriptors with electrocatalytic activity. To enhance predictive accuracy, the team adopted an active learning strategy aimed at minimizing regions of prediction uncertainty. Through clustering analysis, ten candidate structures were selected for subsequent synthesis, iteratively refining the model.

After only forty data points, the improved model (OO-2) achieved prediction uncertainty below the target threshold for all remaining candidates. The OO-2 model predicted $Ca_{0.8}Pr_{0.2}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (CPCF) as a top-performing catalyst with a theoretical OER overpotential of 396 mV; experimental validation confirmed an actual overpotential of 391 mV, surpassing the state-of-the-art $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF).

This study illustrates how uncertainty-aware active learning cycles can be incorporated into SDL frameworks to enable data-efficient exploration of compositional spaces.

5.6. Robotic manipulations

Robotic manipulation serves as a general execution layer that enables physical reconfiguration, module coordination, and parallelized experimentation across autonomous laboratory platforms. Robotic manipulation is a key enabling technology for high-throughput operation in self-driving laboratories, where experimental workflows must be executed and reconfigured with minimal human intervention. In this context, robotic arms serve as integrative execution units that coordinate modular synthesis, processing, and analysis components within dynamically evolving experimental layouts. The robotic manipulation framework highlighted here, led by the team of Dr. Seonghun Hong at the Advanced Institute of Convergence Technology, Seoul National University (Fig. 11), combines robotic arms with reconfigurable modular interfaces that allow rapid exchange and rearrangement of modules and end-effectors. This flexibility supports efficient transitions between sequential and parallel workflows as screening objectives evolve, thereby increasing throughput while reducing downtime. Robotic manipulation is further synchronized with upper-level control software, ensuring that physical operations and experimental recipes are coherently managed in a machine-readable manner. Within autonomous experimentation, this integration positions robotic manipulation as an essential execution layer across materials and chemistry domains.

This direction is also consistent with broader robotics efforts in Korea aimed at coupling advanced manipulation, perception,

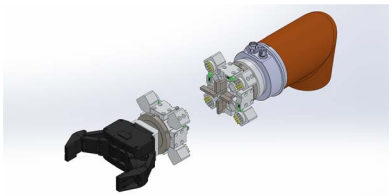

Fig. 11 Robotic manipulation system enabling reconfigurable high-throughput experimental workflows.

and autonomy. For example, KIST's Artificial Intelligence and Robotics Institute encompasses multiple research centers dedicated to AI and robotics, and KIST-affiliated robotics groups within its humanoid/robotics ecosystem have recently pursued projects in high-difficulty autonomous manipulation and fully autonomous smart laboratories. These developments highlight a growing national interest in using intelligent robotic manipulation not only for conventional service or industrial robotics, but also for autonomous experimental systems.[25]

5.7. Agentic AI for higher-level experimentation planner

Recent advances in agentic AI have opened a new direction for autonomous scientific discovery, in which AI systems not only support decision-making but can also coordinate multistep reasoning and workflow execution.[57–59] In the context of SDLs, agentic AI can be viewed as a cognitive layer that links high-level experimental objectives—such as optimizing synthesis conditions or exploring uncharted composition spaces—to the underlying automation infrastructure.[60] In principle, this capability could allow SDLs to move beyond fixed optimization loops toward systems that decompose tasks, integrate heterogeneous information, and iteratively refine experimental plans.

In Korea, early industrial and academic efforts have begun to explore this possibility. For example, LG AI Research has reported agent-based frameworks for accelerating discovery in functional materials and petrochemical R&D, in which foundation models trained on chemical and materials data are coupled with hierarchical decision-making modules to propose candidate synthesis routes or processing conditions.[61] Likewise, Microsoft Korea, in collaboration with domestic manufacturing and energy stakeholders, has introduced agentic AI concepts for digital R&D pipelines that integrate experimental data, simulation outputs, and domain ontologies to support design choices across multiple laboratories.[62] Together, these examples suggest that agentic frameworks may be useful for coordinating heterogeneous digital R&D assets and connecting planning logic with laboratory execution. However, such efforts should presently be interpreted as early-stage demonstrations in constrained settings, rather than as evidence of broadly deployed "virtual scientist" systems.

In the near term, the most realistic role of agentic AI in SDLs is therefore as a decision-support and coordination layer. Such systems can assist with experimental planning, integration of heterogeneous tools, summarization of prior results, and prioritization of next experiments within predefined objectives and safety constraints. In this sense, agentic AI can extend existing Bayesian optimization or active-learning workflows by helping connect planning logic with orchestration software and laboratory metadata, while still operating within human-defined search spaces. By contrast, a more ambitious, longer-term vision is that agentic AI could support higher-level scientific autonomy by generating hypotheses, proposing multistep experimental programs, adapting plans across domains, and interacting continuously with automated laboratory infrastructure. Under this vision, the agent would function not simply as an optimizer, but as a broader scientific planning layer capable of coordinating discovery workflows across materials, chemistry, and bioengineering.

At present, however, several important limitations prevent this longer-term vision from being broadly realized. These include robustness to distribution shifts and unexpected experimental states, reliable uncertainty estimation and validation, safe recovery from hardware and software failures, traceable reasoning and explainability of proposed actions, and consistent enforcement of safety constraints during closed-loop execution. For these reasons, near-term agentic systems in SDLs should be positioned as human-supervised decision-support tools with explicit guardrails, rather than as fully autonomous scientific agents. As validation practices, interoperable datasets, and orchestration frameworks mature, progressively higher levels of autonomy may become feasible.

6. Industrial implementation

The preceding sections highlighted representative SDL applications in Korea and the cross-cutting capabilities that enable them. This section turns to their translation into larger-scale public and industrial R&D environments, where the value of SDLs is increasingly evaluated in terms of throughput, reproducibility, safety, and deployability under real operating constraints. In Korea, SDL principles are extending beyond academia into industrial and government research institutions, signaling a transition toward larger-scale autonomous R&D ecosystems.

The principles of SDLs are extending beyond academia into industrial and government research institutions in Korea, signaling a transition toward larger-scale autonomous R&D ecosystems. At the Korea Institute of Materials Science (KIMS), an autonomous laboratory has been established for alloy development.[63] Robotic arms perform sample placement, followed by arc melting and tube furnace annealing. Samples are then transferred to XRD instruments for phase characterization, and acquired data are processed through reinforcement learning algorithms that iteratively refine process parameters.[63] This system demonstrates feasibility of integrating AI optimization with robotic experimentation in a closed-loop materials development cycle.

In the private sector, LG Chem has launched robotic laboratories to accelerate polymer and catalyst development.[64] These facilities adopt SDL-inspired workflows to enhance throughput, reduce operator error, and streamline data acquisition pipelines, reflecting growing recognition that SDL approaches can

shorten R&D cycles while improving reproducibility, safety, and scalability.

At the Korea Institute of Energy Research (KIER), Minhye Yoon and her team developed a smart laboratory that automates synthesis, analysis, and reaction evaluation.[65] The system targets safety risks in repetitive and hazardous synthesis tasks and aims to bridge laboratory-scale experimentation with industrial process transfer. By integrating XRD instruments with robotic handling, the team established a 24-hour autonomous analysis platform, achieving more than a threefold increase in throughput compared with manual analysis. A QR-based sample management program tracks experiments, while accumulated data are stored in a centralized database with real-time visualization capabilities.[65]

In a notable industrial-academic collaboration, a KAIST-POSCO Holdings platform exemplifies translation of academic SDL frameworks into an industrial environment.[19] The platform is being deployed with an identical configuration, enabling automated synthesis, characterization, and data-driven decision-making workflows established in the laboratory to be utilized without re-engineering. Based on performance demonstrated in the academic setting, this deployment is expected to deliver up to a 93% reduction in materials discovery time by accelerating DRX screening and enabling early identification of high-potential compositions.[19]

Collectively, these developments show that Korea's industrial ecosystem is embracing SDL principles not only for efficiency and safety but also for data-centric innovation.

7. Future prospects of SDLs in Korea

Korea's SDL ecosystem is expanding rapidly, propelled by governmental initiatives and industrial interest. The Ministry of Trade, Industry, and Energy has articulated a national plan to introduce 500 autonomous laboratories by 2030, underscoring the country's ambition to institutionalize SDLs at scale.[12] Market forecasts project the domestic laboratory automation sector to grow from USD 125.8 million in 2024 to USD 320 million in 2035, representing a CAGR of 7.46%.[13]

Yet challenges persist. High initial investment costs restrict SDL deployment to well-funded institutions, leading to uneven adoption. In the private sector, limited awareness of AI's transformative potential has constrained investment, with skepticism regarding near-term profitability. Furthermore, the absence of standardized protocols and interoperability frameworks hinders cross-institutional integration.[66]

Ongoing efforts aim to address these barriers. Academic projects such as ModuFlow and OCTOPUS OS[52] are pioneering modularization and orchestration frameworks, while the K-MDS initiative seeks to standardize data structures across laboratories. Combined with government-backed strategies for AI-driven R&D, these initiatives represent concrete steps toward overcoming technical, cultural, and economic barriers. As discussed in Section 5.4, near-term progress is likely to benefit from layered standardization of (i) device/service interfaces, (ii) structured provenance and metadata, and (iii) workflow semantics and exception/event logging.

8. Conclusions

As demonstrated across nanomaterials, organic/inorganic synthesis, and bioengineering, Korea's SDL efforts are beginning to deliver tangible results. Autonomous platforms have been deployed to synthesize nanoparticles, assemble coin cells, optimize reaction conditions, and manufacture drug-loaded nanoparticles. Software frameworks such as OCTOPUS OS[52] and ModuFlow, together with vision-based safety systems like DenseSSD,[53] are laying groundwork for robust orchestration.

Nevertheless, Korea's SDL journey is still at a formative stage. Key obstacles—including high capital costs, lack of standardized protocols, and limited industrial investment—must be addressed to realize full-scale adoption. Practical interoperability bottlenecks at the level of experimental provenance, workflow semantics, and exception/event logging remain central hurdles for multi-institution scaling and dataset reuse.

Ultimately, Korea's combination of industrial-grade precision hardware and expanding software/data infrastructure positions it uniquely to accelerate SDL development. By fostering collaborations across academia, industry, and government—and by investing in interoperability and validated autonomy—Korea can help shape global standards for autonomous experimentation and strengthen links between discovery and production.

Conflicts of interest

There are no conflicts to declare.

Author contributions

J. H. and S. K. contributed equally to this work. Conceptualization (organizers)—Y. J., J. R., J. P., J. N., J. C.; writing (original draft)—J. H., S. K., S. L., J. K., Se. L., S. M., J. S., J. L., S. H., J. H. H., Y.-S. C., D.-H. S., S. S. H., K. G. K., S.-H. Y., J. H. S., J. C., J. N., J. P., J. R., Y. J.; writing (review & editing)—J. C., J. N., J. P., J. R., Y. J.; project administration—J. R., Y. J.

Data availability

This perspective does not report new experimental datasets. Nevertheless, the SDL platforms described in this manuscript generate structured, provenance-rich experimental records by logging input conditions and contextual metadata (*e.g.*, recipe/protocol versions, environment and instrument settings, and action/event traces) together with measurement outputs (*e.g.*, cycling/EIS, UV-vis spectra, inline FT-IR signals, and particle/drug-loading metrics). Such machine-actionable records can facilitate cross-laboratory benchmarking and downstream reuse when curated and aligned with shared schemas and repository requirements.

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Notes and references

1 G. Tom, S. P. Schmid, S. G. Baird, Y. Cao, K. Darvish, H. Hao, S. Lo, S. Pablo-García, E. M. Rajaonson, M. Skreta, N. Yoshikawa, S. Corapi, G. D. Akkoc, F. Strieth-Kalthoff, M. Seifrid and A. n. Aspuru-Guzik, *Chem. Rev.*, 2024, **124**, 9633–9732.
2 J. T. Rapp, B. J. Bremer and P. A. Romero, *Nat. Chem. Eng.*, 2024, **1**, 97–107.
3 N. J. Szymanski, B. Rendy, Y. Fei, R. E. Kumar, T. He, D. Milsted, M. J. McDermott, M. Gallant, E. D. Cubuk, A. Merchant, H. Kim, A. Jain, C. J. Bartel, K. Persson, Y. Zeng and G. Ceder, *Nature*, 2023, **624**, 86–91.
4 N. Yoshikawa, Y. Asano, D. N. Futaba, K. Harada, T. Hitosugi, G. N. Kanda, S. Matsuda, Y. Nagata, K. Nagato, M. Naito, T. Natsume, K. Nishio, K. Ono, H. Ozaki, W. Shin, J. Shiomi, K. Shizume, K. Takahashi, S. Takeda, I. Takeuchi, R. Tamura, K. Tsuda and Y. Ushiku, *Digital Discovery*, 2025, **4**(6), 1384–1403.
5 J. Li, C. Ding, D. Liu, L. Chen and J. Jiang, *Digital Discovery*, 2025, **4**(7), 1672–1684.
6 A. D. Adesiji, J. Wang, C. S. Kuo and K. A. Brown, *Digital Discovery*, 2026, **5**, 14–27.
7 M. B. Rooney, B. P. MacLeod, R. Oldford, Z. J. Thompson, K. L. White, J. Tungjunyatham, B. J. Stankiewicz and C. P. Berlinguette, *Digital Discovery*, 2022, **1**(4), 382–389.
8 The portion of aged population in Korea, https://kosis.kr/eng/.
9 Birth rate change from korea government, https://www.index.go.kr/unity/potal/main/EachDtlPageDetail.do?idx_cd=1428.
10 K. J. Park H, W. K. Min, H. S. Chi, J. Q. Kim and D. W. Kim, *J. Clin. Pathol.*, 1998, **18**(3), 494–500.
11 Korea Trade-Investment Promotion Agency, https://www.investkorea.org/ik-kr/bbs/i-112/detail.do?ntt_sn=491227.
12 Strategy for AI-powered Innovation and Industrial Data Activation, https://www.fomek.or.kr/main/policy/law/policy_view.php?wr_id=1089.
13 South Korea Laboratory Automation Market, https://www.marketresearchfuture.com/reports/south-korea-laboratory-automation-market-50056.
14 ESG Economist- Batteries have a key role to play if they have low carbon footprintshttps://www.abnamro.com/research/en/our-research/esg-economist-batteries-have-a-key-role-to-play-if-they-have-low-carbon.
15 A. Joshi, D. K. Mishra, R. Singh, J. Zhang and Y. Ding, *Appl. Energy*, 2025, **386**, 125546.
16 D. Han, C. Cui, K. Zhang, Z. Wang, J. Gao, Y. Guo, Z. Zhang, S. Wu, L. Yin, Z. Weng, F. Kang and Q.-H. Yang, *Nat. Sustain.*, 2022, **5**, 205–213.
17 H.-G. Lee, J. Han, M. Kwon, H. Kwon, J. Park, H. J. Hah and D.-H. Seo, *Digital Discovery*, 2026, DOI: 10.1039/D5DD00580A.
18 D.-H. Seo, Accelerating Sodium Solid Electrolyte Discovery, publicly disclosed webinar, https://events.bizzabo.com/771802.
19 KAIST and POSCO Build Autonomous AI Lab for Battery Material Discovery, https://www.ai-newss.com/news/articleView.html?idxno=28327.
20 S. W. Park, H. Kim, S. Han, K. S. Kim, Y. Y. Song, H. G. Lee, W. Jang, D. H. Lee, S. Bae, D. Kim, J. Park, I. Park, S. C. Nam, H. Kim, J. Lee, K. Kang and D. H. Seo, *Adv. Energy Mater.*, 2025, **15**(48), e03496.
21 H.-Y. Chen, M. K. F. Lo, G. Yang, H. G. Monbouquette and Y. Yang, *Nat. Nanotechnol.*, 2008, **3**, 543–547.
22 Y. Guo, M. Wang, Q. Zhu, D. Xiao and D. Ma, *Nat. Catal.*, 2022, **5**, 766–776.
23 M. Chen, W. Luo, Z. Xu, X. Zhang, B. Xie, G. Wang and M. Han, *Nat. Commun.*, 2019, **10**, 4024–4029.
24 M. A. Islam, Y. Xu, W. Tao, J. M. Ubellacker, M. Lim, D. Aum, G. Y. Lee, K. Zhou, H. Zope, M. Yu, W. Cao, J. T. Oswald, M. Dinarvand, M. Mahmoudi, R. Langer, P. W. Kantoff, O. C. Farokhzad, B. R. Zetter and J. Shi, *Nat. Biomed. Eng.*, 2018, **2**, 850–864.
25 H. J. Yoo, N. Kim, H. Lee, D. Kim, L. T. C. Ow, H. Nam, C. Kim, S. Y. Lee, K. Y. Lee, D. Kim and S. S. Han, *Adv. Funct. Mater.*, 2024, **34**, 2312561.
26 B. Burger, P. M. Maffettone, V. V. Gusev, C. M. Aitchison, Y. Bai, X. Wang, X. Li, B. M. Alston, B. Li, R. Clowes, N. Rankin, B. Harris, R. S. Sprick and A. I. Cooper, *Nature*, 2020, **583**, 237–241.
27 Y. Gao, K. Sheng, T. Bao and S. Wang, *J. Pharmaceut. Biomed. Anal.*, 2022, **221**, 115040.
28 Q. T. Easter and S. A. Blum, *Acc. Chem. Res.*, 2019, **52**, 2244–2255.
29 T. Ha, D. Lee, Y. Kwon, M. S. Park, S. Lee, J. Jang, B. Choi, H. Jeon, J. Kim, H. Choi, H.-T. Seo, W. Choi, W. Hong, Y. J. Park, J. Jang, J. Cho, B. Kim, H. Kwon, G. Kim, W. S. Oh, J. W. Kim, J. Choi, M. Min, A. Jeon, Y. Jung, E. Kim, H. Lee and Y.-S. Choi, *Sci. Adv.*, 2023, **9**, eadj0461.
30 Y. Jia, R. Frydrych, Y. I. Sobolev, W.-S. Wong, B. Prajapati, D. Matuszczyk, Y. Bilgi, L. Gadina, J. C. Ahumada, G. Moldagulov, N. Kim, E. S. Larsen, M. Deschamps, Y. Jiang and B. A. Grzybowski, *Nature*, 2025, **645**, 922–931.
31 P. Schwaller, T. Laino, T. o. Gaudin, P. Bolgar, C. A. Hunter, C. Bekas, A. A. Lee and A. C. S. Cent, *Sci*, 2019, **5**, 1572–1583.
32 M. Sacha, M. Błaż, P. Byrski, P. Dąbrowski-Tumański, M. Chromiński, R. Loska, P. Włodarczyk-Pruszyński and S. Jastrzębski, *J. Chem. Inf. Model.*, 2021, **61**, 3273–3284.
33 I. V. Tetko, P. Karpov, R. Van Deursen and G. Godin, *Nat. Commun.*, 2020, **11**, 5575.
34 S. Chen and Y. Jung, *Nat. Mach. Intell.*, 2022, **4**, 772–780.
35 S. Chen and Y. Jung, *JACS Au*, 2021, **1**, 1612–1620.
36 S. Chen, S. An, R. Babazade and Y. Jung, *Nat. Commun.*, 2024, **15**, 2250.
37 S. Chen and Y. Jung, *J Cheminform*, 2024, **16**, 83.

38 S. Chen, R. Babazade, T. Kim, S. Han and Y. Jung, *Sci Data*, 2024, **11**, 863.
39 E. Kim, Z. Jensen, A. van Grootel, K. Huang, M. Staib, S. Mysore, H.-S. Chang, E. Strubell, A. McCallum, S. Jegelka and E. Olivetti, *J. Chem. Inf. Model.*, 2020, **60**, 1194–1201.
40 O. Kononova, H. Huo, T. He, Z. Rong, T. Botari, W. Sun, V. Tshitoyan and G. Ceder, *Sci. Data*, 2019, **6**, 203–211.
41 E. R. Antoniuk, G. Cheon, G. Wang, D. Bernstein, W. Cai and E. J. Reed, *npj Comput. Mater.*, 2023, **9**, 155.
42 J. Jang, G. H. Gu, J. Noh, J. Kim and Y. Jung, *J. Am. Chem. Soc.*, 2020, **142**, 18836–18843.
43 S. Kim, Y. Jung and J. Schrier, *J. Am. Chem. Soc.*, 2024, **146**, 19654–19659.
44 J. Jang, J. Noh, L. Zhou, G. H. Gu, J. M. Gregoire and Y. Jung, *Matter*, 2024, **7**, 2294–2312.
45 S. Kim, J. Schrier and Y. Jung, *Angew Chem. Int. Ed. Engl.*, 2025, **64**, e202423950.
46 G. H. Gu, J. Jang, J. Noh, A. Walsh and Y. Jung, *npj Comput. Mater.*, 2022, **8**, 1–8.
47 J. Choi, S. Kim and Y. Jung, *J. Am. Chem. Soc.*, 2025, **147**, 39113–39122.
48 S. Kim, J. Noh, G. H. Gu, S. Chen and Y. Jung, *Chem. Sci.*, 2024, **15**, 139–145.
49 A. Mottafegh, J.-U. Joo, G.-S. Na, V. Sharma and D.-P. Kim, *Chem. Eng. J.*, 2024, **500**, 157454.
50 H. Noh, N. Lee, G. S. Na and C. Park, *Advances in Neural Information Processing Systems*, 2024, **37**, 25375–25400.
51 G.-N. Ahn, J.-H. Kang, H.-J. Lee, B. E. Park, M. Kwon, G.-S. Na, H. Kim, D.-H. Seo and D.-P. Kim, *Chem. Eng. J.*, 2023, **453**, 139707.
52 H. J. Yoo, K.-Y. Lee, D. Kim and S. S. Han, *Nat. Commun.*, 2024, **15**, 9669.
53 L. C. O. Tiong, H. J. Yoo, N. Kim, C. Kim, K.-Y. Lee, S. S. Han and D. Kim, *npj Comput. Mater.*, 2024, **10**, 42.
54 Y. Sverchkov and M. Craven, *PLoS Comput. Biol.*, 2017, **13**, e1005466.
55 Q. Wei, Y. Wang, G. Yang, T. Li, S. Yu, Z. Dong and T.-Y. Zhang, *npj Comput. Mater.*, 2025, **11**, 10–14.
56 J. Moon, W. Beker, M. Siek, J. Kim, H. S. Lee, T. Hyeon and B. A. Grzybowski, *Nat. Mater.*, 2024, **23**, 108–115.
57 T. Song, M. Luo, X. Zhang, L. Chen, Y. Huang, J. Cao, Q. Zhu, D. Liu, B. Zhang, G. Zou, G. Zhang, F. Zhang, W. Shang, Y. Fu, J. Jiang and Y. Luo, *J. Am. Chem. Soc.*, 2025, **147**, 12534–12545.
58 Y. Zou, A. H. Cheng, A. Aldossary, J. Bai, S. X. Leong, J. A. Campos-Gonzalez-Angulo, C. Choi, C. T. Ser, G. Tom, A. Wang, Z. Zhang, I. Yakavets, H. Hao, C. Crebolder, V. Bernales and A. Aspuru-Guzik, *Matter*, 2025, **8**, 102263.
59 A. M. Bran, S. Cox, O. Schilter, C. Baldassari, A. D. White and P. Schwaller, *Nat. Mach. Intell.*, 2024, **6**, 525–535.
60 S. Kim, J. Choi, K. Jang, J. Park, V. Bernales, A. Aspuru-Guzik and Y. Jung, *arXiv*, preprint: arXiv.2601.15743, 2026, DOI: 10.48550/arXiv.2601.15743.
61 Introducing Agentic AIhttps://v.daum.net/v/20250930155048430.
62 Industrial innovation by Agentic AIhttps://news.microsoft.com/source/asia/2025/09/25/korea-frontier-firms-with-agentic-ai/?lang=ko.
63 Ai Driven autonomous research system developmenthttps://www.kims.re.kr/v17/bbx/board.php?bx_table=05_01%26wr_id=715%26page=2.
64 LG Chem Robot Automation Laboratoryhttps://www.lg.co.kr/media/release/29390.
65 Resolving hazardous and complicated catalyst experiments through Ai-automation System, https://energium.kier.re.kr/sub040101/articles/view/tableid/news/category/2/id/6338.
66 A Policy Blueprint for Unlocking AI's Potential in South Koreahttps://www.kiet.re.kr/en/pub/economyDetailView?detail_no=3016.