**Showcasing Japan's advancements in self-driving laboratory development. Left: Maholo LabDroid from RIKEN Center for Biosystems Dynamics Research, Hyogo, Japan. Right: Robotic powder grinding system from The University of Osaka, Osaka, Japan.**

Self-driving laboratories in Japan

This perspective highlights Japan's initiatives in self-driving laboratory (SDL) development, showcasing diverse applications across materials science, biology, chemistry, and software. In addition, it covers national funding programs, research communities and ecosystems, and industries supporting progress in this field. Additionally, the perspective emphasizes the critical roles of education, standardization, and benchmarking in fostering the continued growth of SDL research.

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# Self-driving laboratories in Japan

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Self-driving laboratories (SDLs) are transforming the scientific discovery process worldwide by integrating automated experimentation with data-driven decision-making. Japan, known for its automation industry, is actively contributing to this field. This perspective introduces Japan's efforts in SDL development, including diverse applications across materials science, biology, chemistry, and software. In addition, it covers national funding programs, research communities, and Japanese industries supporting progress in this field. It also highlights the importance of education, standardization, and benchmarking for the future growth of SDL research.

## 1 Introduction

Self-driving laboratories (SDLs)[1] are transforming the process of scientific discovery. It involves the automation of experiments for large-scale data generation and data-driven decision-making for efficient exploration of the candidate space. As global interest in SDLs continues to grow, Japanese researchers are actively contributing to the field. This perspective offers an overview of research efforts related to SDLs in Japan.

Japan has been renowned for its advanced automation technology, holding a 46% share of the global industrial robot market as of 2023.[2] This background has fostered an affinity for laboratory automation research, where robots often play a central role. In 1988, Matsuda *et al.* demonstrated the optimization of reaction conditions using an automated system.[3] This system can be considered as one of the earliest SDLs in Japan, as it incorporates a laboratory robot with decision-making by the simplex method. A fully automated laboratory system for testing blood samples built by a Japanese hospital in the 1980s is reported by Sasaki *et al.*[4] Their approach gained global attention as a promising method to reduce laboratory testing costs.[5]

The development of SDLs could offer valuable solutions to address Japan's social challenges, particularly its declining birth rate and shrinking workforce. This demographic shift has created a need for innovative solutions to maintain productivity

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with fewer people. SDLs can reduce the burden of labor-intensive experimental work in laboratories, enabling research to continue with fewer staff members. Additionally, SDLs improve researchers' work-life balance, an increasingly important consideration in Japan's work culture. Moreover, Japan's demographic shift threatens the transmission of technical expertise to future generations. SDLs can help preserve the specialized knowledge of experienced professionals by automating tasks and replicating their skills. While these advantages are particularly relevant to Japan, other countries facing similar demographic trends may also benefit from SDLs in the near future.

The remainder of this paper is structured as follows. To introduce the current state of automation in Japan, we provide a review of Japanese SDLs across three application areas—materials science, biology, and organic chemistry in Section 2 to 4. Section 5 explores the software aspects of SDLs by introducing research efforts on AI for scientific discovery. Section 6 highlights national funding programs to promote advancements in automation-focused studies. Section 7 addresses the activities to form research communities and ecosystems. An overview of the Japanese industries supporting SDL development is provided in Section 8. Finally, Section 9 discusses the future directions of SDLs, and Section 10 concludes the paper. The geographical locations of SDLs introduced in this article are shown in Fig. 1. This perspective is based on a workshop held at the Institute of Science Tokyo in October 2024.

## 2 Materials science

The materials industry is a key sector of Japan's economy, and active research in materials science is being conducted there. As part of the government's strategy to strengthen materials innovation, data-driven research methods are actively promoted through projects like the DxMT.[6] This section reviews efforts in Japan to advance SDLs in materials science. Section 2.1 outlines an automated system for synthesizing and evaluating thin-film materials. Section 2.2 provides an overview of the MaiML format, a standardized data format for measurement analysis instruments. Section 2.3 details a robotic experiment setup for discovering electrochemical materials. Section 2.4 and 2.5 highlight autonomous polymer synthesis achieved by two research groups. Section 2.6 explores the development of

radiative cooling materials. Applications of robot arms for mechanochemical synthesis and autonomous X-ray diffraction analysis are covered in Section 2.7. Finally, Section 2.8 introduces Process informatics.

### 2.1 Autonomous experiments for thin-film materials

Thin-film research is important for a wide range of fields, including semiconductor devices, sensors, catalysts, optics, and various coatings. Shimizu, Hitosugi, and colleagues reported a closed-loop system for inorganic thin-film materials in 2020.[7] The system combines Bayesian optimization, automated synthesis, and automated physical property evaluation (Fig. 2(a)). The system consists of a robot arm positioned at the center of a hexagonal chamber, which is connected to six satellite chambers with an automated sputter thin-film synthesis equipment and an automated electrical resistance evaluation system (Fig. 2(b)). The robot arm handles all sample transfers between the satellite chambers. Autonomous experiments aimed at minimizing the electrical resistance of Nb-doped $TiO_2$ thin films achieved a throughput 10 times higher than manual methods.[7] Furthermore, the system discovered a novel electrolyte material for all-solid-state Li batteries. Specifically, by mixing $Li_3PO_4$ and $Li_{1.5}Al_{0.5}Ge_{1.5}(PO_4)_3$ (Fig. 2(c)), an amorphous thin film ($Li_{1.8}Al_{0.03}Ge_{0.05}PO_{3.3}$) shows higher Li-ion conductivity than either of the original materials [$Li_3PO_4$ and $Li_{1.5}Al_{0.5}Ge_{1.5}(PO_4)_3$] (Fig. 2(d)).[8]

To reduce the number of experiments in the Bayesian optimization process, the hyperparameters of the kernel and acquisition functions were tuned.[9,10] Leveraging the knowledge and expertise of materials researchers is essential for tuning.
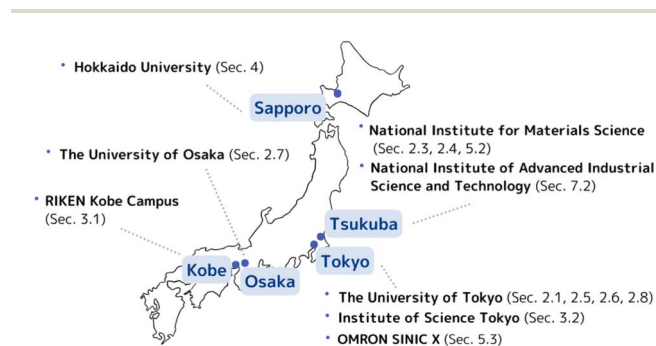
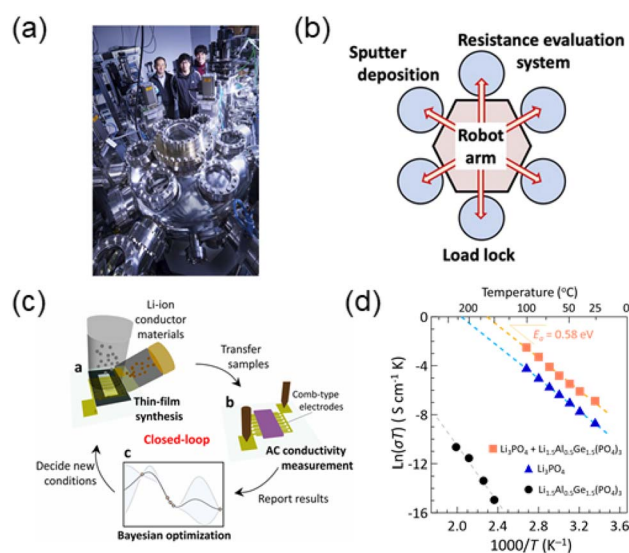**Fig. 1** Geographical locations of SDLs introduced in this article.

**Fig. 2** (a) Photograph and (b) schematic of autonomous experimental system for exploration of inorganic thin-film materials. Copyright 2020 Shimizu et al.[7] and reprinted with permission under CC BY 4.0. (c) Autonomous experimental cycle for exploration of ionic conductors. (d) Ionic transport properties of fabricated amorphous ionic conductors thin films. Reprinted with permission from Kobayashi et al.[8] Copyright 2023 American Chemical Society.

For example, materials researchers can anticipate the process window of synthesis parameters and the scale of changes in physical properties, which is the key to tuning the values of hyperparameters.

Since this system can connect multiple measurement and analysis instruments, it can acquire various physical properties from multiple aspects to generate big data. For this purpose, a standardized measurement and analysis data format (Measurement Analysis Instrument Markup Language: MaiML) was applied to the system.[11] The format is described in the next section. For interested readers, a review on autonomous experimental systems in materials science is available from Ishizuki et al.[12]

## 2.2 Standardization of data format with MaiML

Representing data in a standardized, structured format is crucial for facilitating automated analysis by computers. Various data formats have been developed to store different types of information. For example, Chemical Description Language ($\chi$DL) has been introduced to describe experimental procedures in organic chemistry.[13] Currently, measurement instruments from different manufacturers often provide data in different formats. This lack of a standard format requires users to convert the formats manually or to prepare data conversion software. Therefore, there is a strong need for a standard format. In response, the Japan Analytical Instruments Manufacturers Association (JAIMA), in collaboration with its member companies and the Ministry of Economy, Trade, and Industry (METI), established a data format called the Measurement Analysis Instrument Markup Language (MaiML). In May 2024, MaiML was registered as a Japanese Industrial Standard (JIS K 0200).

The MaiML format was developed as a standardized data format with independent availability to achieve an instrument-agnostic data structure. The format follows the findable, accessible, interoperable, and reusable (FAIR) data principles.[14] An XML format describes the processes of measurement, pre-processing, and postprocessing steps. Detailed descriptions of sample fabrication processes and measurement conditions ensure the reproducibility of experiments. Additionally, logs for each measurement operation provide traceability. The format also includes tamper-prevention features and data encryption capabilities. These features allow MaiML to encompass essential information for the reproducibility of sample fabrication to measurement and analysis, thus contributing to database construction (Fig. 3). Guidelines for MaiML are available on **https://www.maiml.org/**.

## 2.3 High throughput robotic experiments for rechargeable batteries

Data-driven automated robotic experiments are an effective method to accelerate the development of new-materials even in the field of rechargeable batteries.[15] Specifically, optimizing the composition of electrolytes and identifying effective additive combinations involves evaluating an enormous number of potential candidate materials.[16] Historically, this process has
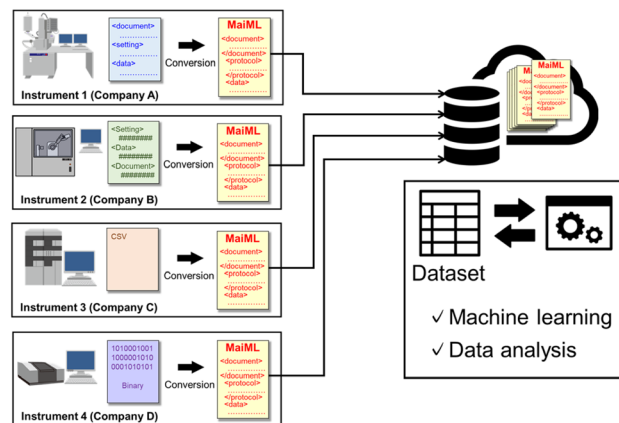


Fig. 3 Schematic of the utilization of the standardized data format of Measurement, Analysis, Instrument Markup Language (MaiML).

relied heavily on trial-and-error approaches, leading to significant bottlenecks in the development of new electrolyte materials.

To overcome these challenges, Matsuda et al. developed the robotic experimental setup for searching electrochemical materials discovery using high-throughput combinatorial techniques by use of miniaturized microplate type electrochemical cells.[17] The system consisted of a liquid handling dispenser and a 96-channel electrochemical analyzer equipped with a robotic microplate handling arm, with a search throughput of over 1000 samples per day. By integrating with Bayesian optimization techniques, they discovered the specific composition of electrolyte that enhances the cycle life of lithium-oxygen batteries,[18] demonstrating its effectiveness in significantly accelerating the identification of optimal electrolyte compositions (Fig. 4). A key feature of their system is its



**Automated Robotic Experiment**

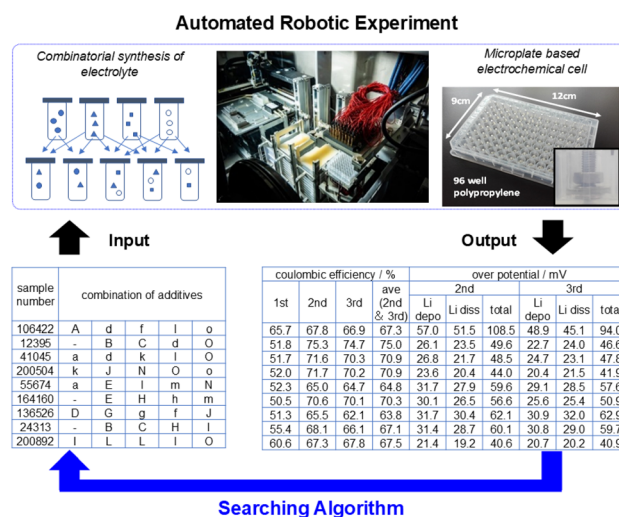| sample number | combination of additives | | | | | coulombic efficiency / % | | | | over potential / mV | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | 1st | 2nd | 3rd | ave (2nd & 3rd) | 2nd | | | 3rd | | |
| | | | | | | | | | | Li depo | Li diss | total | Li depo | Li diss | total |
| 106422 | A | d | f | l | o | 65.7 | 67.8 | 66.9 | 67.3 | 57.0 | 51.5 | 108.5 | 48.9 | 45.1 | 94.0 |
| 12395 | - | B | C | d | O | 51.8 | 75.3 | 74.7 | 75.0 | 26.1 | 23.5 | 49.6 | 22.7 | 24.0 | 46.6 |
| 41045 | a | d | k | l | O | 51.7 | 71.6 | 70.3 | 70.9 | 26.8 | 21.7 | 48.5 | 24.7 | 23.1 | 47.8 |
| 200504 | k | J | N | O | o | 52.0 | 71.7 | 70.2 | 70.9 | 23.6 | 20.4 | 44.0 | 20.4 | 21.5 | 41.9 |
| 55674 | a | E | I | m | N | 52.3 | 65.0 | 64.7 | 64.8 | 31.7 | 27.9 | 59.6 | 29.1 | 28.5 | 57.6 |
| 164160 | - | E | H | h | m | 50.5 | 70.6 | 70.1 | 70.3 | 30.1 | 26.5 | 56.6 | 25.6 | 25.4 | 50.9 |
| 138526 | D | G | g | f | J | 51.3 | 65.5 | 62.1 | 63.8 | 31.7 | 30.4 | 62.1 | 30.9 | 32.0 | 62.9 |
| 24313 | - | B | C | H | I | 55.4 | 68.1 | 66.1 | 67.1 | 31.4 | 28.7 | 60.1 | 30.8 | 29.0 | 59.7 |
| 200892 | I | L | L | l | O | 60.6 | 67.3 | 67.8 | 67.5 | 21.4 | 19.2 | 40.6 | 20.7 | 20.2 | 40.9 |

Fig. 4 Schematic illustration of the data-driven high-throughput automated robotic experiments for searching multi-components electrolyte for rechargeable batteries. Figure adapted with permission from Matsuda et al.[18] Copyright 2022, Elsevier.

autonomous exploration capability, which is achieved with the use of NIMO, an automation software for establishing a closed-loop workflow between artificial intelligence and robotic experimentation.[19] The details of NIMO are described in Section 5.2. Recently, the group extended their interest for practical design of battery cells, and reported the development of fully automated sequential robotic experimental setup for the cell fabrication of stacked-type battery cells with fabrication throughput over 80 cells per day, which is 10 times higher than conventional human-based experiments.[20]

## 2.4 Advances in autonomous synthesis for polymers

Autonomous synthesis in polymer science has progressed significantly since the early 2000s, with high-throughput (HTP) techniques driving advances in polymerization. Early developments focused on automating polymer synthesis processes, particularly for combinatorial studies, to enhance speed and reproducibility.[21] A major milestone was the application of automation to precision-controlled polymerization, such as Reversible Addition–Fragmentation Chain Transfer (RAFT) and Atom Transfer Radical Polymerization (ATRP). These techniques allow precise control over polymer architecture, molecular weight, and functionality, enabling the creation of complex and customized polymers.[22,23] HTP methodologies have facilitated the rapid creation of polymer libraries and optimization of synthesis parameters, though dataset sizes remain a limitation. Recent innovations in platforms like Chemspeed have replicated most manual processes, integrating Python-based tools like Chemspyd[24] for real-time adaptive control and process optimization.

Despite these advancements, challenges persist in characterizing critical physical properties, such as mechanical and thermal performance. For example, tensile testing for adhesive materials requires specialized setups and skilled sample preparation. Addressing this, Naito and Sato developed a high-throughput testing system for adhesives, which uses miniaturized specimens to provide more realistic performance metrics while reducing material usage.[25] Moreover, integrating machine learning techniques, such as Bayesian optimization, with flow synthesis has enabled autonomous experiments for optimizing radical polymerization.[26,27] In summary, while autonomous synthesis has revolutionized polymer research, the integration of automation and intelligent algorithms promises further advancements, addressing current challenges and unlocking new possibilities for material innovation.

## 2.5 Flexible lab-automation using robot arms for polymer materials development

Polymer materials are widely used in academia and industry. Most polymer materials used for actual products are in the form of composites to reinforce multi-functionality, for instance by being mixed with dielectric fillers. However, automation in the development processes of polymer composite materials is still limited because of the challenges in handling materials in the form of powders and granules and molding processes required for property characterization and application.

A Japanese team has been developing an automated system for polymer materials development. One of the sub-processes is the press process (Fig. 5(A)).[28] A robot arm was adopted to construct a system that handles the tools for the operations, such as press plates and forks, and to increase the flexibility of the system for future adaptability rather than built-in automation of a dedicated system. The control software operates both the robots and the press machines. An experimental closed loop was formed to obtain effective press parameters and evaluates the thickness of the polymer film by image processing and press parameters. Another automated sub-process is the property measurement systems (Fig. 5(B)), such as the one for a dielectric property utilizing the force-sensing capability of a robot arm for stabilization of polymer placement.[29] The automated system successfully measured the dielectric properties with the same accuracy as trained humans.

The flexibility of the system was enhanced by the use of a gripper interface that enables the grasping of multiple tools and thus the completion of complex pressing processes with a single robot arm. The same type of robot arms was used in both the press and measurement sub-processes. The use of a single type of robot arm reduces the development and maintenance costs for an automated workflow than the development of multiple dedicated automation machines for each process.

## 2.6 Automated film development system generating massive data for radiative cooling

Amid growing concerns over urban heat islands, sky radiator technology, which selectively emits thermal radiation in the
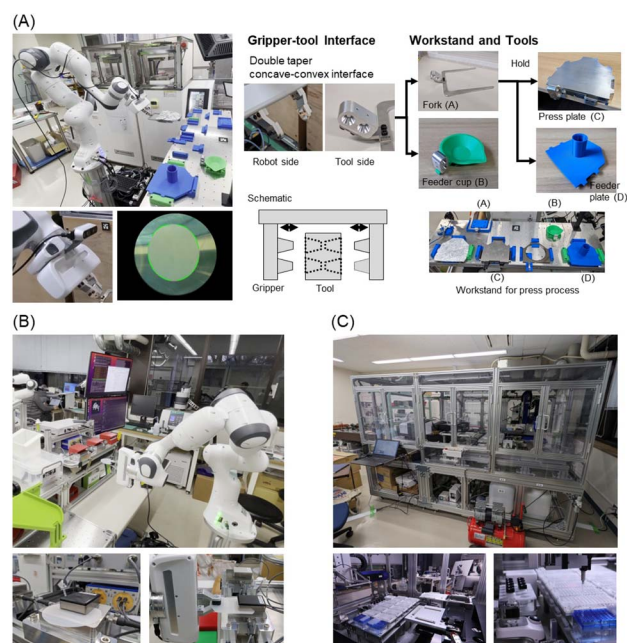


**Fig. 5** (A) Press process automation system for polymer materials development, adapted from Asano *et al.*[28] (B) Dielectric property measurement system. Reprinted with permission from Asano *et al.*[29] Copyright 2024, IEEE. (C) Automation system for heat transfer materials development.

atmospheric window region (8–13 μm) to directly radiate heat into outer space, has received significant attention. Shiomi *et al.* have been developing thermal radiative metamaterials by combining electromagnetic field analysis and machine learning to optimize metamaterials, achieving high-performance thermal emitters.[30,31] While metamaterials are advantageous in the wavelength selectivity of radiation, the difficulty in fabrication poses a significant barrier to widespread application.

As a scalable and cost-effective approach to developing radiative coolers, they are working on organic–inorganic hybrid coatings consisting of a polymer matrix and inorganic fillers. The thermal radiation properties in the atmospheric window region and the solar reflection properties in the visible range for heat shielding depend on the optical absorption of the polymers and inorganic fillers themselves, along with the resonances and scattering phenomena occurring at their interfaces. Consequently, the parameter space becomes extremely large because it incorporates not only material parameters, such as the type and mixing ratio of polymers and inorganic fillers, but also process parameters, such as casting and drying conditions. For example, a coating involving five materials and three process parameters, such as mixing time, casting speed, and drying temperature, yields an 8-dimensional search space. Exploring just 10 choices per parameter results in $10^8$ combinations, leading to a combinatorial explosion. To address this challenge with high throughput, they are developing an automated coating system capable of producing 1000 coatings per day under various conditions and automatically acquiring infrared and visible reflection spectra (Fig. 5(C)). Additionally, they have developed a spectral prediction model, useful for controlling radiative properties, using a dataset of over 10 000 data.

## 2.7 Robotic mechanochemical synthesis and autonomous XRD analysis

Mechanochemical synthesis, which induces chemical reactions through mechanical force, offers an energy-efficient, solvent-free method for producing materials such as metal–organic frameworks (MOFs) and energy-related compounds. However, traditional methods like manual grinding or ball milling often struggle with reproducibility and control. To overcome these challenges, Nakajima *et al.* developed a force-controlled robotic mechanochemical synthesis system,[32] combined with an autonomous X-ray diffraction (XRD) analysis workflow[33] (Fig. 6). This system not only provides precise control over grinding force and speed but also enables automated, high-throughput structural analysis through autonomous XRD.

In their experiments with perovskite materials, the robotic synthesis system demonstrated superior reproducibility compared to manual and ball milling methods, especially for force-sensitive reactions. By adjusting the grinding force and speed, they could significantly influence the reaction pathways, allowing for precise control of reaction outcomes. For instance, increased grinding force produced higher yields of $Cs_4PbBr_6$, while variations in speed shifted the reaction toward other phases like $CsPbBr_3$.
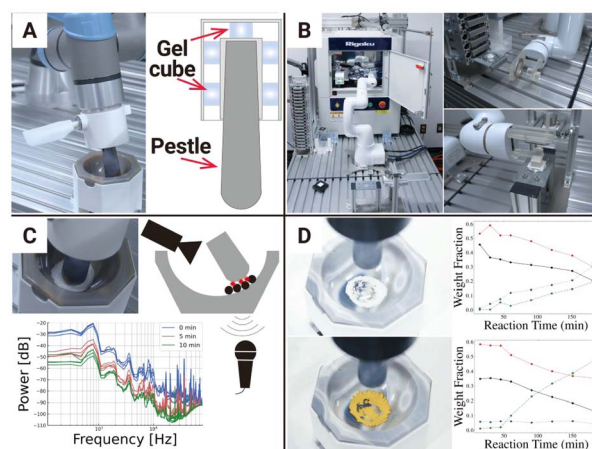


Fig. 6 Automated system for powder material experiments. (A) Robotic powder grinding system using a Soft Jig, where the jig's softness ensures safe grinding without the need for force sensing. (B) Autonomous powder X-ray diffraction system for preparing XRD samples and performing automated Rietveld analysis. (C) Enhanced robotic powder grinding using visual and audio feedback, with grinding sounds providing particle size information for more efficient grinding. (D) Robotic mechanochemical synthesis controlling reaction pathways through force conditions applied by a pestle.

Once the synthesis was complete, the fully autonomous XRD system seamlessly handled sample preparation, measurement, and data analysis. This integration allowed for high-throughput analysis and minimized human error, particularly in the reproducibility of low-angle diffraction patterns, which are crucial for characterizing materials like lead halide perovskites.

This combined robotic synthesis and autonomous XRD approach offers a powerful tool for both advancing the understanding of reaction mechanisms and accelerating the discovery of novel materials. Future work will explore the application of this system to a wider range of materials.

## 2.8 Process informatics – robotic objective process exploration system (ROPES)

In order for new materials to be incorporated into final products, process development and production technology development are necessary, and AI robot-driven development is also effective (Fig. 7(a)). Process Informatics is located downstream of Materials Informatics. Experimental-based Bayesian optimization was demonstrated in the powder-film-dying process of a catalyst layer in polymer electrolyte fuel cells (PEFCs).[34]

The catalyst layer of a solid polymer electrolyte fuel cell is composed of carbon as an electronic conductor, fluoropolymer as a proton conductor, pores in the gas diffusion space, and platinum nanoparticles as a reaction catalyst. The arrangement of the three-dimensional microstructure changes significantly depending on how it is applied and dried, and optimization is required. The autonomous experiment system shown in Fig. 7(b) discovered new drying-process parameters among $8^5$ candidates with 40 trials minimizing the defect ratio (Fig. 7(c)). Not only the high-throughput exploration but also five process
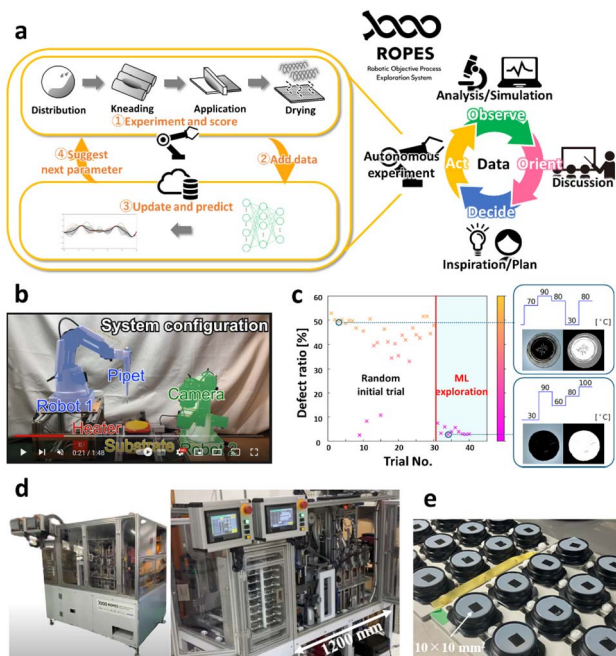
**Fig. 7** ROPES of powder-film-formation-process, (a) schematic of an autonomous system, (b) experimental setup with two robot hands,[36] (c) results of exploration of drying process parameters minimizing defect ratio,[34] (d) a scalable autonomous system, (e) high-throughput prototyped fuel cell catalyst layer samples. A video about ROPES is available online.[35]



**Fig. 8** The LabDroid Maholo including peripheral equipment. Reprinted from Kanda et al.[38] under CC BY 4.0.

routes were found. Furthermore, we also prototyped an elevator-sized autonomous system as shown in Fig. 7(d), which can automatically demonstrate factory processes, *i.e.*, die-coating and zone-heating, and evaluate defect ratio, but also micron-sized surface roughness and electronic impedance. The small-sized samples are prototyped with various process parameters (Fig. 7(e)). A video demonstration of this system is available online.[35]

Process informatics is a methodology for process exploration using small amounts of prototyped material samples, which will lead to the accelerated social implementation of incorporation into final products.

## 3 Biology

Automation in biological experiments has been pursued across various fields and processes. For example, PCR experiments—widely recognized due to COVID-19 testing—had already begun transitioning from manual water bath operations to automated thermal cyclers by the late 1980s.[37] Numerous specialized instruments like automated pipetting systems have been developed, significantly improving the efficiency of fixed operations. However, more versatile robotic systems are needed, especially for automation in basic research. In Japan, the versatile humanoid robot Maholo LabDroid, developed by Yaskawa Electric Corporation and the Robotic Biology Institute Inc., is widely used from fundamental to clinical research (Fig. 8).
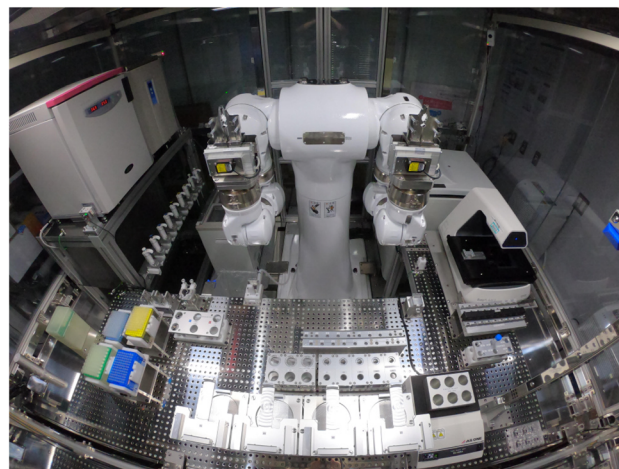
### 3.1 Maholo LabDroid

Maholo LabDroid has been employed in molecular and cellular biology, drug screening, culturing and immunostaining of induced pluripotent stem cells (iPS cells), and in closed-loop cell culture using AI and robotics.[39–43] By combining this robot with optimization AI, Kanda *et al.*, have successfully conducted autonomous experiments targeting cell cultures for regenerative medicine.[38] Specifically, they used a batch Bayesian optimization algorithm with LabDroid Maholo to autonomously explore combinations of seven parameters—such as reagent concentrations, processing times, and cell handling intensities—involved in differentiating iPS cells into retinal cells, achieving efficient induction without human intervention. Beyond basic research, Maholo LabDroid is also utilized in clinical studies. A research team at Kobe City Eye Hospital created a sterile environment by integrating the robot with a clean booth and successfully transplanted cells cultured by the robot into patients during clinical research on retinal cells.[44] As of October 2024, Maholo LabDroid is not sold outside Japan.

### 3.2 Robotic crowd biology

A Japan-led team has proposed the concept of Robotic crowd biology in 2017, which involves aggregating hundreds of robots into a robotic experimentation center for cloud-based experiments.[45] Researchers submit their desired experimental protocols to the center *via* a network, where AI and robots efficiently execute the experiments and return the results. This approach offers various benefits, such as improving the reproducibility and traceability of scientific experiments, fundamentally resolving research misconduct, increasing the utilization rates of expensive advanced equipment, and efficiently conducting high-biosafety-level experiments. Ultimately, it envisions making biological research widely accessible to all humanity.

In the Robotic Crowd Biology concept, managing numerous robots and devices makes it impractical for humans to instruct each one individually. To address this, the development of AI

and software for directing robots is actively underway. A research team at the University of Tsukuba has developed algorithms to achieve parallel scheduling necessary for efficiently operating multiple robots.[46,47] While some scheduling algorithms exist in the field of factory automation (FA), the authors' formulation considers time constraints specific to life science experiments—such as reaction times and the degradation of living cells and reagents—that are set among processes. To automate the monitoring of multiple devices that would otherwise require human oversight, the same team developed image recognition software, fine-tuned for identifying labware used in life science experiments, to monitor the status of labware placed inside automated dispensing robots.[48] Additionally, a research team at RIKEN has demonstrated that it is possible to automatically convert experimental procedures written in natural language into robot-operating code using large language models.[49] Furthermore, the development of AI-based systems to manage robots and experimental equipment from higher levels is currently being extensively pursued. Supporting these efforts, a prototyping lab has been established at RIKEN BDR in Kobe, and a demonstration facility is planned at the Institute of Science Tokyo. In recent years, researchers outside Japan have also begun exploring ways to take advantage of a cloud-based experimental platform, spurring discussions and initiatives worldwide toward its realization.[50]

# 4    Organic chemistry

In organic chemistry research, experimental procedures still largely depend on researchers' expertise and manual operations. However, there is a continuous demand for more efficient alternatives to these traditional methods, resulting in the development of various innovative approaches. Recently, automated synthesis robots have drawn significant attention for their potential to automate and even autonomously conduct organic chemistry research. Utilizing these robots can achieve high reproducibility and experimental precision, offering substantial improvements in efficiency compared to conventional manual processes. This technological advancement simplifies labor-intensive synthetic experiments and considerably reduces the workload of researchers.

In the field of organic synthesis, two primary types of robots are commonly employed: articulated robots and Cartesian coordinate robots. Here, articulated robots are highly flexible, with multiple joints that enable complex, multi-directional movements. This makes them ideal for intricate tasks, such as transferring reaction vessels, adjusting equipment, and performing precise reagent additions in confined spaces. In contrast, Cartesian coordinate robots operate along fixed linear axes, making them well-suited for high-precision, repeatable tasks like liquid handling, reagent dispensing, and automated sample preparation with minimal positioning errors. Many processes in organic synthesis can often be segmented into simple operations that are well-suited for execution by Cartesian coordinate robots. For example, the polymerization of poly(quinoxaline-2,3-diyl)s *via* living polymerization of diisocyanobenzene derivatives has been successfully automated

using a Cartesian coordinate robot.[51,52] In this process, the resulting polymer thin films were reported to exhibit unique selective reflection behavior. It was found that even slight inaccuracies in the monomer composition and variations in the degree of polymerization had a significant impact on the selective reflection wavelength. Therefore, precise control of these parameters was critically important. In particular, it was necessary to dispense volumes with an accuracy of less than $10 \mu L$. However, in the early 2010s, among the commercially available automated systems investigated in the study, no articulated robot was known to achieve this level of dispensing precision with organic solvents. Consequently, a Cartesian robot (Chemspeed SWING) was employed for this purpose.

Additionally, direct integration of Cartesian coordinate robots with various analytical instruments is under active investigation. For instance, integration with a UV-visible-NIR spectrophotometer has enabled the development of a solubility prediction model for porphyrins,[53] while integration with chromatography systems has facilitated the automatic evaluation of asymmetric catalysts, advancing the development of a high-performance catalyst.[54] More recently, combining robots, chromatography systems, and the PHYSBO package introduced in Section 5.2 has been explored for autonomous optimization of chemical reaction conditions.[55]

Beyond commercial laboratory automation systems, low-cost hardware is crucial for reducing the entry barrier to SDLs.[56] Kuwahara *et al.* developed a 3D-printed robot named FLUID to democratize automation in materials synthesis.[57] They showed its utility by demonstrating the coprecipitation of cobalt and nickel to form binary materials. All design files and control software are released under an open-source license, allowing users to modify and adapt the system to their own research environments.

# 5    AI for science

Since SDLs involve the automation of data-driven decision-making,[1] SDL research requires developing intelligent software as well as automation hardware. In this section, we review the software side of SDLs in Japan, focusing on the field of AI for science. The foundation models for material discovery developed in IBM Research-Tokyo are described in Section 5.1. Black box optimization software packages developed by Japanese teams are introduced in Section 5.2. Research by OMRON SINIC X is covered in Section 5.3 and several applications of large language models for scientific research are outlined in Section 5.4.

## 5.1    Foundation models for material discovery

The integration of AI models into self-driving laboratories enhances their capabilities, enabling the preselection of promising materials before chemical synthesis and guiding experiments to achieve desirable properties. Property prediction and structural generation are particularly promising AI applications. However, traditional AI models developed by individual research groups within specific material domains are often

limited in size and small training datasets (order of 10 to 100 samples), resulting in insufficient modeling accuracy.

To address these limitations, recent advancements inspired by large language models (LLMs) have been adopted in materials informatics. These approaches involve pre-training large models in a self-supervised manner using massive datasets. Such pre-trained models effectively capture general material representations and can be fine-tuned with small domain-specific datasets for various downstream applications. Examples of foundation models include MolCLR,[58] a GNN-based architecture pre-trained with 10 million molecular samples, and ChemBERTa,[59] which uses the RoBERTa architecture pre-trained with 77 million SMILES samples. Although these models perform well in regression and classification tasks, their single-modal nature leaves room for improvement. Recent studies explore multi-modal representations of materials to enhance modeling capabilities. Shirasuna et al.[60] introduced models that fuse SMILES and molecular graphs using a Mixture-of-Experts approach, achieving superior performance over single-modal models. As noted in Takeda et al.,[61] multi-modal modeling is an emerging field with vast opportunities, including efficient fusion methods and strategic modality selection. Other modalities, such as SELFIES, 3D atom positions, electron density, optical spectra, and text descriptions, are also under consideration. These foundation models can significantly enhance SDL capabilities by utilizing their predictive and generative functions, enabling the design of more promising candidate materials. For instance, ref. 62 demonstrates how a SMILES-based foundation model was integrated into a human-in-the-loop workflow connected to an SDL. Similarly, as demonstrated by RoboRXN,[63] synthetic pathways predicted by a foundation model can be executed in automated robotic laboratories. Some of these models are openly accessible on GitHub[64] and Hugging Face, encouraging open development within the materials informatics community. Specifically, Foundation Model for Materials (FM4M) has achieved widespread adoption through active community-building efforts through the AI Alliance,[65] bridging academia and industry toward shared innovation goals.

## 5.2 Black box optimization methods and NIMO

Black box optimization techniques are useful as an AI to suggest experimental conditions to be tested, which can be the brain of self-driving labs (Fig. 9). Bayesian optimization is probably the best-known technique for achieving desired material properties. The Python packages COMBO (COMmon Bayesian optimization)[66] and PHYSBO (optimization tool for PHYSics based on Bayesian optimization)[67] can quickly perform the Bayesian optimization calculations. On the other hand, there are various needs in materials research, but also the improvement of material properties, and other techniques are required. For example, to construct phase diagrams with a small number of experiments, the Python package PDC (Phase Diagram Construction) has been developed by adopting the uncertainty sampling strategy.[68] To visually explore phase diagrams using PDC, a web application called AIPHAD (Artificial Intelligence
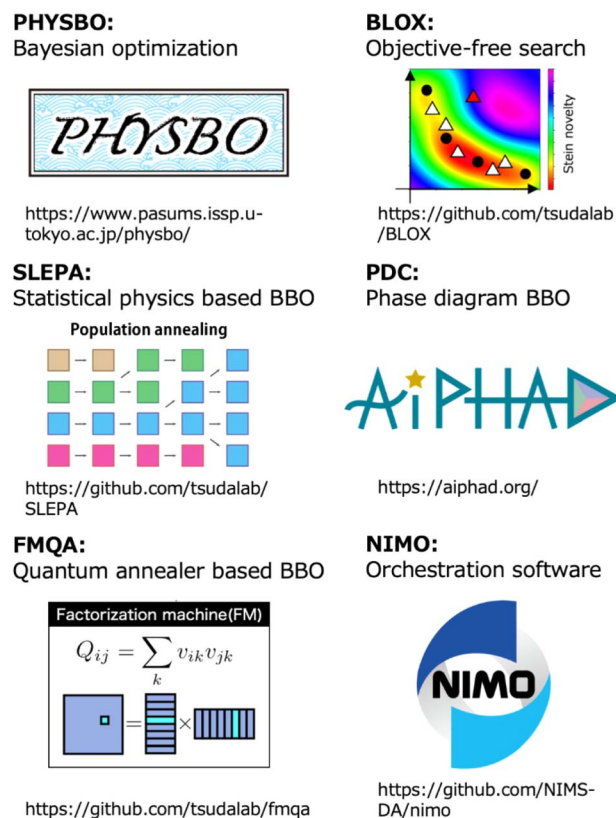


**Fig. 9** Black box optimization methods depending on the aim of exploration. Reprinted from ref. 71–73 under CC BY 4.0.

techniques for PHAse diagram) is freely available.[69,70] In addition, algorithms such as BLOX (BoundLess Objective-free eXploration)[71] for overlooking the material property spaces and SLEPA (Self-Learning Entropic Population Annealing)[72] for obtaining the material property distributions with the small number of experiments have been developed as open source software. Furthermore, the black box optimization technique using quantum annealer and Ising machines called FMQA (Factorization Machine with Quantum Annealing) has been developed to explore vast material space.[73] Although these methods have been mainly developed in materials science, we believe that they can be used not only in materials science but also in any self-driving labs for biology, organic chemistry, etc.

To achieve a self-driving lab by combining the robotic experimental devices introduced in Section 2.3 and three black-box optimization techniques (PHYSBO, PDC, and BLOX), a generic software NIMO (NIMS Orchestration System) has been developed.[19,74] In NIMO, a robotic experiment and a black-box optimization method are treated as modules, and the system is designed to enable various autonomous automated material explorations by selecting these modules. As a demonstration experiment, autonomous automated experiments on electrolytes for lithium metal electrodes were carried out using the robotic experimental setup for searching electrochemical materials discovery (see Section 2.3) controlled by NIMO. As a result, a total of 384 electrolytes were successfully developed

as autonomous automated experiments without human intervention using NIMO. Globally, various types of orchestration software (OS) have been developed.[75–77] NIMO has an advantage over other OSs due to its focus on AI algorithms, particularly its use of diverse black-box optimization methods, beyond Bayesian optimization. These methods are designed to be easily integrated into other OSs, allowing us to enhance the capabilities of self-driving laboratories by combining NIMO with other systems. Additionally, we are developing new AI algorithms to address a range of exploration needs. By incorporating these into NIMO, we aim to establish it as an evolving open-source software (OSS). Furthermore, the three algorithms already implemented in NIMO are widely used in materials science,[78] chemistry,[79] and drug discovery,[80] leveraging both experimental and simulation data. Thus, we believe that NIMO can facilitate interactions between these different domains in Japan.

### 5.3 From foundation model to AI scientist

As discussed in Section 5.1, foundation models are being developed across various fields, with comprehensive applications being considered for SDLs. These applications extend beyond providing scientific knowledge in respective fields; related to Section 5.2, LLMs can also encompass optimization tasks,[81] and as will be discussed in Section 5.4, they include a series of research activities such as hypothesis generation, experimental design and implementation, paper writing, and reflective review as AI scientist.[82]

OMRON SINIC X Corporation, a research subsidiary of OMRON that focuses on healthcare and factory automation, is advancing various projects utilizing foundation models in AI and robotics to realize real-world AI scientists. Following the philosophy of OMRON's founder, "To the machine, the work of the machine, to man the thrill of further creation", the company has been researching how to understand and support human creation through AI and robots. A particular focus has been understanding human research and experimental work, conducting research and development through open innovation with universities and public research institutions while receiving competitive research funding.

The company's research into understanding research data encompasses several key streams. The first focuses on law discovery, which involves tackling the symbolic regression problem to discover scientific laws between variables from measured data.[83] This machine learning challenge takes tabular data containing variable values as input and outputs mathematical formulas showing relationships between variables.[84] The second stream involves map-based visualization, primarily targeting materials science, where representation learning techniques are applied to various data types including material structures, measurement data, and property-describing text.[85] The goal is to create visualizations where materials with similar properties are mapped close to each other. The third stream concentrates on novel material design[86] and property prediction,[87] including research on generating new crystal structures and developing Transformer architectures to predict properties of crystal structures with unknown characteristics.

Regarding the reproduction of experimental work, much of the robotics research has focused on powder manipulation. Powders present more challenging handling requirements than liquids in terms of weighing, grinding, and mixing, making them an engaging research topic in robotics. For instance, research on powder-weighing robots has achieved sub-milligram precision in lifting and dropping powder using spoons through simulation-based learning.[88] In powder grinding research, efficient powder processing has been achieved by utilizing multiple modalities of information, including visual and vibration data.[89]

In parallel, research is being conducted on AI robots that can execute various tasks while understanding environmental data and linguistic instructions.[90] Future plans involve connecting the above-mentioned AI for research understanding with experimental automation robots, advancing this research to realize AI robot scientists capable of conducting real-world experiments.

### 5.4 Large language models for automated scientific research

LLMs have been adopted by multiple SDLs[91,92] because of their powerful ability in natural language processing. A number of applications on LLM for automated scientific research have been released from Japan. Sakana AI, a Japan-based startup, proposed the AI Scientist,[82,93] which aims for fully automatic scientific discovery by harnessing the power of LLMs. Hatakeyama-Sato et al. explored the ability of GPT-4 in various chemical tasks and elucidated their current limitations.[94] They also applied GPT-4 for parameter selection of a polymer property prediction[95] and a semiautomated system for synthesizing polyamic acid particles.[96] Jiang et al. developed ProtoCode,[97] a tool that can extract protocol information from natural language text and convert it to intermediate representation formats. They demonstrated its ability by generating thermal cycler operation files from polymerase chain reaction (PCR) protocols written in natural language. Machi et al. developed a framework for reviewing the results of automated conversions of structured organic synthesis procedures extracted from the literature.[98] In this framework, organic synthesis procedures in the literature are transformed into a structured chemical description language ($\chi$DL)[13] using both a proposed rule-based method and a generative large language model-based method.[91] The results from both methods are presented simultaneously to users, facilitating efficient transformation and refinement.

As the potential of LLMs has become widely recognized, the race for their development has intensified. Both commercial models, such as GPT-4,[99] and open-weight models like LLaMA[100] and DeepSeek,[101] are now widely available. To support the development of LLMs in Japan, the Ministry of Economy, Trade and Industry (METI) and the New Energy and Industrial Technology Development Organization (NEDO) started the Generative AI Accelerator Challenge (GENIAC)[102] in February 2024. The government-funded project subsidizes the computational costs of LLM training for the selected players. The first term (February–August 2024) supported 10 projects including Sakana AI's, and the second term (October 2024–April 2025) selected 20 projects including 3 projects about LLMs for medicine.

# 6 AI-robot-driven science

Japan Science and Technology Agency (JST), one of the major national funding agencies for science, supports multiple projects related to SDL research. Two JST-Mirai projects, Accelerating Life Sciences by Robotic Biology,[103] Materials Exploration space Extension Platform (MEEP),[104] and two JST Moonshot projects, Co-evolution of Human and AI-Robots to Expand Science Frontiers[105] and AI & Robots that Harmonize with Humans to Create Knowledge and Cross Its Borders[106] collaboratively founded the AI-Robot-Driven Science Initiative[107] in 2023 to promote the new scientific methodology realized by AI and robotics. In 2024, "Research innovation through autonomous-driven research systems" has been designated as one of the strategic objectives authorized by the Ministry of Education, Culture, Sports, Science and Technology (MEXT),[108] and a new funding program "R&D Process Innovation by AI and Robotics"[109] has been started. In this section, we introduce these government-supported projects on AI-robot-driven science.

## 6.1 Accelerating life sciences by robotic biology

This project, part of JST-Mirai Program in the "Common Platform Technology, Facilities, and Equipment" area, addresses critical issues in life sciences—such as low reproducibility, inefficient use of costly equipment, research misconduct, and the labor-intensive nature of laboratory work—through advanced laboratory automation. While laboratory automation tools are increasingly available, most are limited to specific tasks, still relying on human operators to manage samples, reagents, and data interpretation. Consequently, human error and labor remain constraints on the effectiveness of automation. This project aims to overcome these limitations by developing a comprehensive suite of technologies. These include a standardized experimental protocol description language and IoT-based systems architectures designed for the coordinated operation of diverse robotic and automated equipment. The project's application areas broadly span the biological sciences, including proteomics, genome editing, and stem cell culture. This interdisciplinary effort involves leading institutions like RIKEN, AIST, University of Tsukuba, and major industry partners including YASKAWA Electric and TECAN Japan. The project began with a feasibility study (2018–2020) and moved to full-scale development in 2021, with completion anticipated in March 2025. Funded at approximately 1.1 billion yen (∼7.3 million USD), this initiative strives to redefine experimental workflows, minimizing human involvement and enhancing reproducibility and operational efficiency across the life sciences. Many of the project's outcomes are presented in Section 3.1 (Maholo LabDroid) and 3.2 (Robotic crowd biology).

## 6.2 Materials exploration space extension platform

MEEP was launched in the JST-Mirai project in 2021.[110–112] Researchers' experiment and intuition are important in materials research and development (R&D), and the researchers' inspiration should be more effectively utilized by AI and robot

systems. MEEP's proof of concept is 1000 times throughput of exploration of ion-conductive materials for solid-state batteries. The materials exploration space is overwhelmingly expanded in R&D sites with the following three methods;

(1) High-throughput autonomous exploration systems;

● "make": Autonomous prototyping system with vacuum coating[7–9]

● "measure": "Materials doc" including autonomous crystal analysis system[113]

● "save": materials property prediction system[114]

(2) Data-driven/hypothesis driven hybrid system (Fig. 10);

OODA loop with "make"–"measure"–"save"–"understand" induces inspiration[85]

(3) Knowledge sharing;

The knowledge obtained from the data is shared among R&D institutes, R&D companies, and measuring instrument manufacturers.

## 6.3 Co-evolution of human and AI-robots to expand science frontiers

In the current movement toward scientific automation through AI and robotics, the focus is largely on conducting reproducible, high-throughput experiments to accelerate scientific discoveries. However, such automation proves effective primarily when hypotheses can be tested at low cost and within a short time frame, and when experiments involve repetitive actions on rigid objects. As experimental models become increasingly complex, hypothesis testing generally requires greater investment of both time and resources. For instance, in life sciences, experiments with high-fidelity model organisms—far more complex than cell-based tests—pose significant challenges for automation. These organisms are typically small, flexible, and variable, limiting the ability of current robotics to perform precise experimental procedures based solely on pre-programmed instructions.
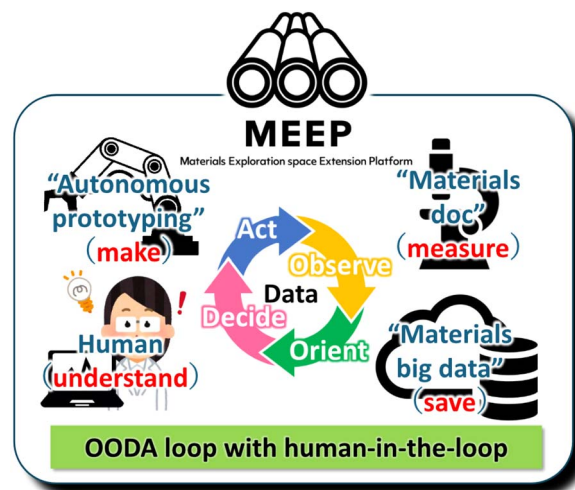


Fig. 10 Schematic of MEEP policy based on OODA loop. Observe phase: materials doc, orient phase: materials big data, decide phase: human, act phase: autonomous prototyping.

In scenarios that demand experimentation in extreme environments where each task cannot be pre-specified, autonomous robots capable of self-directed learning and action become essential. Such autonomy allows robots to leverage their unique ability to reconfigure physical capabilities, presenting a novel, robotics-specific approach to scientific exploration. This project under JST Moonshot Goal 3 aims to realize autonomous AI robotic scientists by 2050. Through transdisciplinary research, it integrates mathematical foundations, scientific AI, robotic AI, and robotic hardware.

### 6.4 AI & robots that harmonize with humans to create knowledge and cross its borders

This project aims to develop AI robots that can harmonize with humans to create knowledge and transcend its boundaries by 2050. The initiative represents a significant advancement in the integration of artificial intelligence with scientific research and innovation processes.

The project has established clear milestones, with the first target set for 2025: developing AI robots capable of understanding, reproducing, and explaining research conducted by human scientists, while also generating novel hypotheses. By 2030, the project envisions these AI robots collaborating with researchers across various fields to drive innovation, resulting in the publication of peer-reviewed papers. The ultimate goal for 2050 is to create an environment where researchers and AI systems can work together to produce Nobel prize-level research achievements.

The research framework encompasses three interconnected components. The experiment automation AI robot system is designed to conceptualize experiments based on research hypotheses, estimate specific procedures in cyberspace, and execute them in physical space. This includes developing automated synthesis capabilities and understanding experimental papers. The Claim and analysis AI focuses on comprehending multimodal scientific data and providing language-based evidence, utilizing a foundation model that can understand relationships between research papers and generate comprehensive analyses. The Description and dialogue AI system aims to summarize experimental results and update hypotheses through interactive discussions with researchers, incorporating researcher feedback to improve performance without requiring large datasets.

To achieve these objectives, the project employs various advanced technologies including large language models, multimodal AI systems, and automated synthesis devices. The project particularly emphasizes the importance of combining deductive thinking for continuous performance improvement with inductive thinking and abduction for paradigm disruption, ultimately aiming to create a new approach to scientific discovery that leverages both human expertise and artificial intelligence capabilities.

### 6.5 Research process innovation with AI and robot

As a public funding program related to self-driving laboratories in Japan, the "R&D Process Innovation by AI and Robotics:

Technical Foundations and Practical Applications" field was launched by the JST in 2024. This funding primarily targets young researchers and conducts three phases of three-and-a-half-year research projects, with about 30 research proposals expected to be selected in total. The purpose of this program is to revolutionize the R&D process through the use of AI and robotics. By introducing AI and robotics, the program aims not only to free researchers and engineers from simple tasks but also to enable them to tackle complex challenges beyond conventional cognitive and physical capabilities. It is anticipated that by advancing R&D through collaboration between researchers, engineers, and AI and robotics, unprecedented scientific discoveries and technological innovations will be realized, transforming the nature of R&D. This program seeks proposals from researchers in AI, robotics, and applied fields such as life science and materials science, with the goal of creating foundational technologies that contribute to innovating the R&D process using AI and robotics. By fostering close collaboration among researchers in these fields, the program promotes the construction of methodologies and their practical applications for R&D powered by AI and robotics. By linking foundational technology development with practical applications in scientific and technological research, the program aims to build a general-purpose framework for autonomously driven R&D, creating new scientific discoveries and technological innovations.

## 7 Ecosystem

Collaboration among researchers or industry partners is indispensable for developing SDLs that require experts from various fields. This section reviews the efforts to promote collaboration for SDLs. We introduce Japanese communities for lab automation users and developers in Section 7.1. An initiative in a national research institute for sharing modules is described in Section 7.2.

### 7.1 Community—LASA, LADEC and Digital Laboratory Consortium

In Japan, the Laboratory Automation Suppliers' Association (LASA) was established in May 2019 to accelerate the development of complex laboratory automation systems by fostering a regional community of developers.[115] Recognizing that modern laboratory automation demands expertise across hardware, software, operational management, and application domains, LASA provides a platform where various experts with different backgrounds collaborate closely from the planning stage. Through regular events like the monthly workshop and the annual Laboratory Automation Developers Conference (LADEC), LASA offers opportunities for members to stay updated on the latest developments, share insights, and engage in face-to-face collaborations. These events feature talks, discussions, and activities that cover a broad spectrum of topics, from hardware customization to software and AI development, as well as operational best practices. Several outcomes influenced by collaborations and discussions within that community have been published to date.[43,44,46,47,49,116–120]

As of October 2024, LASA has grown to over 3200 members from academia, industry, government agencies, and media, facilitating cross-disciplinary interactions among researchers, engineers, management, and students. By bridging the gap between diverse fields of expertise, LASA plays a critical role in advancing laboratory automation development in Japan and serves as a model for regional developer communities.

As an organization dedicated to materials science, the Digital Laboratory Consortium[121] was established in September 2023, bringing together more than 40 companies to exchange information and develop technologies for automatic and autonomous experiments.

### 7.2 AUTOkobo at AIST

At the National Institute of Advanced Industrial Science and Technology (AIST) Japan, efforts are underway to increase research efficiency and streamline experimental processes by improving access to laboratory automation. This initiative, called "AUTOkobo," was developed as part of the in-house "Multi-Modal AI" (MMAI) project,[122] which aims to improve digital transformation (DX) literacy among researchers. The MMAI project enables even beginners to develop advanced AI technologies through education and shared programming resources. Recognizing the need for more efficient data acquisition, the AUTOkobo was launched in 2023 and has since expanded to all seven research departments at AIST.

The AUTOkobo focuses on automating traditionally batch-based experimental processes, particularly in areas such as, polymers, inorganic materials, thin films, and ceramics. Central



**Fig. 11** Conceptual image of AUTOkobo infrastructure accelerating SDL development in AIST. Automation modules, such as liquid dispensing or powder dispensing, are developed and shared allowing each SDL to integrate them into their systems to perform complex tasks.

to its approach is the modularization of laboratory processes (Fig. 11, below). Automation modules, such as robots and liquid or powder dispensing devices, are provided free of charge, allowing researchers to integrate them into their workflows to perform complex tasks. In Self-Driving Lab (SDL) systems, robotics and peripherals manage the flow of materials between instruments, while the AUTOkobo team supports system integration to reduce the burden on the researchers. In addition, the AUTOkobo is developing a workspace that serves as both a showroom and a workshop for automation technologies, allowing researchers to engage in hands-on examination of the available modules and instruments. This modular approach addresses key challenges in laboratory automation, including low costs, system flexibility, and integration of new systems into conventional experimental setups. By providing flexible automation modules, researchers can automate experiments without financial risk, and once completed, modules can be reused by others. In this way, the AUTOkobo approach not only saves time and resources but also promotes the widespread adoption of automation across diverse research domains, including polymers, inorganic materials, thin films, and ceramics.

## 8 Industry support for SDL development

Japan has active manufacturing industries, and universities and research institutes often collaborate closely with companies to develop SDLs. This section outlines the contributions of Japanese industries to SDL development and highlights partnerships between academia and industry. Section 8.1 introduces robotic arms developed in Japan, Section 8.2 highlights custom-made automation systems created through collaborations, and Section 8.3 showcases software development efforts.

### 8.1 Robotic arms

Robotic arms play a central role in some SDLs for their dexterity in object handling. Japan has competitive robot manufacturers, including FANUC and YASKAWA, which are two of the "Big 4", the four largest industrial robot manufacturers in the world. They provide different kinds of robot arms for SDLs. For example, Maholo LabDroid (Section 3.1) was developed by YASKAWA and the Robotic Biology Institute. A collaborative robot COBOTTA by DENSO WAVE is adopted in the autonomous X-ray diffraction analysis system[33] (Section 2.7) and a robotic pipetting system for plant pots.[123] Industrial robotic arms from DENSO WAVE are integrated into a multiarm robotic platform for scientific exploration.[124] An industrial robot MELFA from MITSUBISHI ELECTRIC has been incorporated into an automatic gamma-ray activation analysis system at Japan Atomic Energy Agency.[125] A dual-arm robot NEXTAGE from Kawada Robotics has been utilized in the cell culture system in a pharmaceutical company Eisai[126] and powder dispensing system by ExaWizards.[127]

### 8.2 Custom-made lab automation system

SDLs in Japan are often developed through close collaboration between academia and industry. For example, Shimadzu
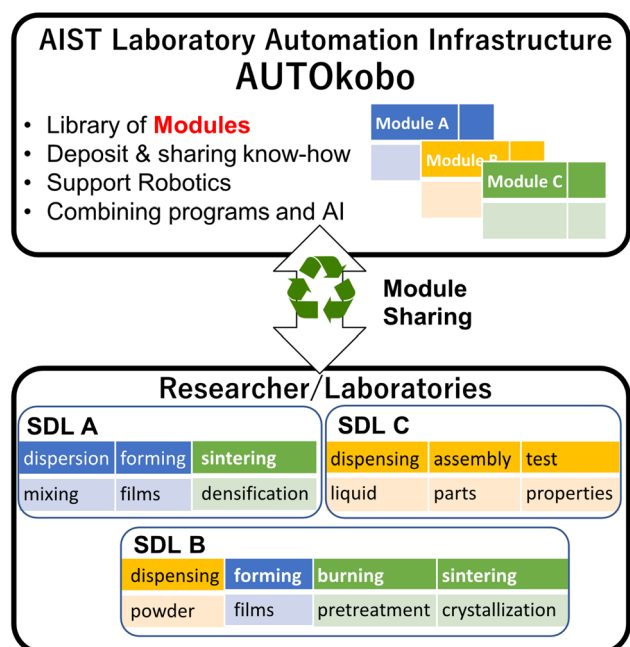
Corporation and Kobe University jointly developed an autonomous laboratory system for biotechnology research and demonstrated the optimization of medium conditions for bacteria to improve glutamic acid production.[128] KiQ Robotics developed Lab Auto, an integrated system that automates RNA evolution experiments at The University of Tokyo.[129] Here, we present three case studies from SDLs developed by the authors to highlight the real-world challenges and their solutions.

The first case study is the Lab Full Automation system from ForDx.[130] The collaboration between ForDX and Furukawa Electric Advanced Engineering Co., Ltd brought expertise in developing automation technology that integrates dispensing and measurement devices. However, they lacked the capability to create a self-driving laboratory by incorporating AI algorithms. To address this, NIMO (Section 5.2) was employed to establish a closed-loop system between experiments and AI, enabling the development and commercialization of self-driving laboratory devices. In Japan, the development of hardware and software for machine learning has traditionally been conducted independently. We recognize that fostering close integration between these two elements is a key challenge for the widespread adoption of self-driving laboratories in Japan.

Another case study is from HORIBA, Ltd that is collaborating with ROPES (Section 2.8). The FC(fuel cell)-ROPES, shown in Fig. 7(d) and (e), was developed by a nationally-funded project by the New Energy and Industrial Technology Development Organization (NEDO) with the initial users from R&D sites at Japanese fuel cell stack OEMs, including Toyota, Honda, Panasonic, and Toshiba. These companies required a higher-throughput system for exploring process parameters that could be applied in real factories. While they were interested in automation, traditional R&D methods based on manual labor were estimated to be more cost-effective compared to automation systems developed independently by individual companies. To overcome this barrier and promote system adoption, it was necessary to reduce the unit price and increase the operating efficiency. To achieve this, the FC-ROPES was designed with three design-philosophies: (i) scalability, including a wide range of process parameters and customizable evaluation units (*e.g.*, customer-selectable objective functions) (ii) desktop size for quick delivery and fast returns and adaptability to project changes, and (iii) the ability to function as a pilot line for real factories. As demand for fuel cells grows and prices decrease, the system can be expanded horizontally to other applications using powder-film-formation processes, such as batteries or ceramic films. Furthermore, when the number of users of the production process R&D increases, commoditization is likely to spread among academic researchers as well.

Finally, Nishio, Hitosugi *et al.* have recently constructed a digital laboratory, called dLab, which interconnects instruments using robots to collect experimental data (including synthesis processes, measured physical properties, and measurement conditions) for solid materials research in thin-film form.[131] Several modular experimental instruments are interconnected (Fig. 12), allowing automated material synthesis, measurement, and analysis. Data from the instruments are output in the MaiML format and stored in a cloud-
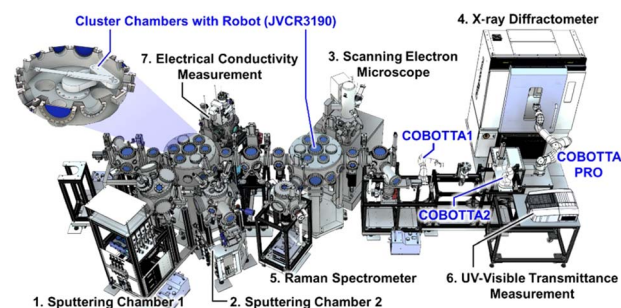


Fig. 12 Schematic of the digital laboratory (dLab) for thin film materials.[131]

based database. JEOL Ltd has developed an automated scanning electron microscope for thin film samples that can be connected to the dLab system (Fig. 12). Rigaku Corp. has developed a thin-film X-ray diffractometer that works with a robot for experiments, both of which are commercially available. Additionally, Shimadzu Corp. and HORIBA, Ltd provide optical properties measurement systems. All these instruments follow established standards for physical connections and communication protocols, which are publicly available.[132] The dLab system autonomously synthesized high-quality $LiCoO_2$ (001) thin films, optimizing the X-ray diffraction peak-intensity ratio using Bayesian methods. The diffraction pattern files in MaiML format on the cloud were automatically analyzed, and Bayesian optimization autonomously proposed the next thin-film deposition condition to obtain better-quality thin films. It showcases advanced autonomous material synthesis driven by data and robotics for materials science.

In addition, companies often collaborate to develop laboratory automation systems. A robotic system for mouse tail vein injection developed by Preferred Networks and Chugai Pharmaceutical[133] is a notable example, which is now commercialized as AUTiv.[134] TORCH, Inc. provides laboratory automation solutions to companies, such as automated pouring and closing of sample containers with collaborative robots at Lion Corporation.[135]

### 8.3 Software development

To realize SDLs, it is important to develop programs to control each device. These programs are implemented in Python, Lab-VIEW, and various other languages. In Japan, there are companies that can help with the development of the control programs of devices. For example, CJS Inc. has created a Lab-VIEW program to control a syringe pump, contributing to developing an automated autonomous odor blending system.[136] Furukawa Electric Advanced Engineering has developed a program for automated dispensing equipment, which has been implemented in the robotic experimental setup for searching electrochemical materials discovery (see Section 2.3).

## 9 For the future of SDLs

We have reviewed the current state of SDLs in Japan. While significant research has been conducted, their adoption

remains limited due to various challenges. Further democratization is necessary for wider adaptation of SDL technologies.[56] This section identifies the key barriers and explores potential strategies to alleviate them, facilitating broader implementation of SDLs.

Adopting SDLs may face several challenges, one of which is a reluctance to change. Many researchers often prefer to rely on traditional methods and hesitate to adopt next-generation strategies, perhaps due to familiarity with traditional methods, technological barriers, lack of trust in the new methodologies, *etc.* This issue can be mitigated through the education of young researchers, particularly during the early stages of their training. Educational efforts in Japan aimed at nurturing future automation developers are introduced in Section 9.1. Another challenge lies in the high cost of hardware and software development. Many current SDLs are monolithic, meaning they are entirely custom-built with non-replaceable components. Standardization plays an important role in reducing costs and enhancing flexibility (modularity and expandability). Standardized interfaces enable modular systems, allowing users to customize setups, select affordable hardware, and optimize their systems based on their requirements. Standardization also allows software reuse. This topic is further explored in Section 9.2. Finally, benchmarks are vital in helping users select appropriate methods and guiding developers in taking their first steps into SDL development. Several benchmarks for SDL research are proposed in Section 9.3 to support this objective.

## 9.1 Education

To enhance the development of SDLs in the future, education programs that familiarize students with the concept of SDLs are necessary. Several lecture courses have already been provided in Japanese universities for this purpose.

At Keio University, a practical training course on AI-robotic science has been offered to undergraduates. As part of the JST-Mirai Program described in Section 6.1, from 2021 to 2024, a 5–6 days intensive course titled "Automation of Scientific Experiments" was conducted using actual robots.[137] The course was designed to allow students to experience how AI connected to experimental robots can discover new knowledge through automated experiments. Specifically, students learned to program experimental protocols for liquid-handling experiments, which are fundamental techniques for PCR tests and chemical experiments—using Python to fully control the OT-2 liquid-handling robot (Opentrons Labworks Inc.). They also built an automated experimental planning AI that interprets results, plans subsequent experiments, and instructs the robot, creating an AI-robot system that autonomously performs scientific experiments. By first manually performing the experimental processes and then implementing them into the robot and AI, students gained a deeper understanding of how the collaboration between humans, automation, and AI can enhance problem-solving capabilities, foster creativity, and improve learning outcomes in addition to their respective roles. Participants ranged from students engaged in life science research to those using a micropipette for the first time, but all were new to programming robots for experiments. Through collaborative learning and tackling assignments, they gained various stimulating experiences. Plans are underway to transfer the course to other universities.

The Department of Chemistry at The University of Tokyo offers Information Chemistry as a regular lecture course, teaching the basics of materials informatics and SDL to third-year undergraduates and above.[138] The lecture also includes hands-on experience with machine learning and teaching robots to perform specific motions. This is a unique lecture in Japan as there are still only a few institutions that can teach robotics in chemistry.[139] At the Institute of Tokyo Science (Science Tokyo), materials informatics can be studied systematically in an organization called TAC-MI; basic education on SDL has also been initiated.[140] These educational efforts can provide young students and potential future researchers with a foundational understanding of new technologies as well as offer a hands-on experience that helps reduce the mental barriers to their adoption.[141]

In addition to lectures at universities, textbooks written in local languages help disseminate knowledge about SDLs to a broader audience. A book entitled 'Intersection of Materials, Machine Learning, and Robotics'[142] has been published to support the development of the community. LASA (see Section 7.1) is also planning to create a textbook on laboratory automation. These resources will be valuable to the field by providing researchers with foundational knowledge and making SDL development more accessible.

## 9.2 Standardization

SDLs typically connect devices such as robot arms and measurement instruments. As automation system requirements change, hardware and software may need replacement. Standardization is crucial for creating flexible systems that allow hardware to be replaced while keeping software changes minimal. Key areas of standardization include hardware dimensions, physical connection interfaces, and communication protocols. Modularity achieved through standardization can lower development costs and encourage broader adoption of SDL technologies.

Several initiatives have been undertaken by various groups to address this need for standardization. For instance, the IVI Foundation provides open industry standard software architectures, including the Virtual Instrument Software Architecture (VISA),[143] which aims to improve the interchangeability of test and measurement instruments that communicate through a variety of I/O buses. Similarly, the SiLA Consortium[144] develops open standards to support the integration of laboratory automation systems. Recently, the Laboratory and Analytical Device Standard (LADS)[145] has been introduced as a manufacturer-independent, open standard for analytical and laboratory equipment. It is built upon Open Platform Communications Unified Architecture (OPC UA) and aims to improve the plug and play interoperability of analytical devices. These efforts involve manufacturers and impact the direction of hardware development.

Japan Analytical Instruments Manufacturers Association (JAIMA) advances the standardization of laboratory and analytical instruments in Japan. JAIMA contributed to the development of LADS OPC UA and the standardization of the MaiML format (Section 2.2) as Japanese Industrial Standards (JIS K 0200).

Although standards play a crucial role in enhancing interoperability, the real challenge lies in ensuring their widespread adoption and compliance. Close collaboration between stakeholders, including academia and industry, is essential to developing practical and effective standards. Additionally, the existence of multiple competing standards may undermine the intended benefits of standardization. To facilitate global adoption, international collaboration is also critical to promoting the broad implementation of these standards.

### 9.3 Benchmark for SDLs

Benchmarks have been helpful for various research areas by facilitating the comparison of different methods, and the need for standard benchmarks for SDLs was highlighted during the authors' meeting. Here we propose potential benchmarking tasks to evaluate the practical utility of lab automation systems to enhance the international discussion on establishing SDL benchmarks.

**9.3.1 Powder dispensing.** In comparison with liquid dispensers, powder dispensing is still tricky because of the complex mechanics of small particles. The use of robotic arms has been investigated recently[88,146] to overcome the limitations of commercial devices such as Chemspeed or Quantos (Mettler Toledo). Due to the widespread nature of the task and the diversity of approaches available, powder dispensing is suitable for a benchmarking task. Benchmark criteria can include speed, accuracy, and hardware cost, allowing researchers to develop robotic systems optimized for specific performance aspects.

**9.3.2 Viscous liquid handling.** Working with viscous liquid is required in various experiments. For instance, this may be the case when using compounds with melting points near room temperature, such as di-*tert*-butyl dicarbonate or tri-*tert*-butylphosphine, as reagents, or when using highly viscous polymers or oligomers as reaction substrates. Furthermore, in industrial production, reducing the amount of solvent often enhances productivity, which frequently necessitates the consideration of high-viscosity, highly concentrated solutions. However, currently available liquid handlers sometimes have difficulties in treating viscous liquids, and optimization of the liquid handling parameters is necessary for desirable performance.[147] Benchmarks on viscous liquid handling would help developers choose an appropriate device for their use case. Polyethylene glycol (PEG) can be used as a viscosity standard because of the diversity in viscosity.

**9.3.3 Robot performance in realistic tasks.** Precise object handling is often required to complete regular tasks in SDLs, such as microplate placing.[148] Although the manufacturers usually provide the repeatability of their robotic arm, this metric does not always reflect their precision in practical applications since various factors, such as payload, can affect

the performance of the robot. Harazono, *et al.*[116] developed a platform to evaluate the microplate handling accuracy of robot arms. Practical benchmarks like this are useful for assessing the real-world performance of robotic systems.

## 10 Conclusions

This perspective has highlighted the advancements in SDL research in Japan, spanning material sciences, biology, and organic chemistry. Furthermore, we have explored the roles of community collaboration, funding initiatives, and the industry that supports the growth of SDLs.

Compared to SDLs developed in other countries, a distinctive characteristic of Japan's SDL development might be the strong collaboration between academia and industry. As discussed in Section 8, universities and national research institutes in Japan frequently partner with industrial collaborators, including small companies, to develop custom automation hardware tailored to specific research needs. In addition to Japan's strong automation industry, active measurement and analysis equipment manufacturers, holding an 8% of the global market share as of 2021 and ranking third after the United States and Germany,[149] are supporting the development of Japanese SDLs. The integral nature of SDLs also aligns with the strengths of Japanese manufacturers, as Japan tends to have a comparative advantage in products with a more integral architecture.[150] However, it has been pointed out that Japanese robotics research is lagging, reflecting the relatively weak performance in the field of AI.[151] Advancements in AI may also be crucial for the further development of SDLs in Japan.

In addition to research institutes, companies also show strong interest in SDLs. Japan has a large concentration of materials, automation, and scientific equipment industries. These companies are making efforts to introduce SDLs to enhance the creativity of researchers. Although the number of SDLs is still small, their use is steadily spreading. By building synergy among diverse players, SDLs in Japan will continue to develop and drive innovation in the field.

## Data availability

As this is a Perspective article, no primary research results, data, software or code have been included.

## Author contributions

Conceptualization (organizers)—D. N. F., T. H., K. Nis., W. S., S. T., K. Tsu., N. Y.; writing (original draft)—Section 1: N. Y.; Section 2.1, 2.2: T. H., K. Nis.; Section 2.3: S. M.; Section 2.4: M. N.; Section 2.5, 2.6: Y. A., J. S., K. S.; Section 2.7: K. O.; Section 2.8: K. Nag.; Section 3: G. N. K., T. N., H. O., K. Tak.; Section 4: Y. N.; Section 5.1: S. T.; Section 5.2: R. T.; Section 5.3: Y. U.; Section 5.4: N. Y.; Section 6.1: K. Tak.; Section 6.2: K. Nag.; Section 6.3: K. H.; Section 6.4: Y. U.; Section 6.5: I. T.; Section 7.1: T. H., G. N. K.; Section 7.2: D. N. F., W. S.; Section 8: T. H., K. Nag., K. Nis., R. T., N. Y.; Section 9.1: T. H., G. N. K., H. O.;

Section 9.2, 9.3, 10: N. Y.; Writing (review & editing)—D. N. F., N. Y.; project administration—N. Y.

## Conflicts of interest

Tohru Natsume is an executive at Robotic Biology Institute Inc., which may benefit financially from the increased scientific use of Maholo LabDroid.

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