Democratization of autonomous chemical and materials research with self-driving labs

Richard B. Canty[1], Jeffrey Bennett[1], Keith A. Brown[2], Tonio Buonassisi[3], Sergei V. Kalinin[4], John R. Kitchin[5], Benji Maruyama[6], Robert G. Moore[7], Joshua Schrier[8], Martin Seifrid[9], Shijing Sun[10], Tejs Vegge[11], Milad Abolhasani[1,*]

[1] Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, North Carolina 27606, United States
[2] Department of Mechanical Engineering, Boston University, Boston, MA, 02215, USA
[3] Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, 02139, MA, USA
[4] Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee 37996, USA
[5] Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, USA
[6] Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433, USA
[7] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831 USA
[8] Department of Chemistry and Biochemistry, Fordham University, The Bronx, New York 10458, USA
[9] Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27695, United States of America
[10] Department of Mechanical Engineering, University of Washington, Seattle, WA 98195, USA
[11] Department of Energy Conversion and Storage, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
* Corresponding Author, E-mail: abolhasani@ncsu.edu

Abstract

In the evolving landscape of scientific research, the complexity of global challenges demands innovative approaches to experimental planning and execution. Self-Driving Laboratories (SDLs) represent a significant advancement in automating not only experimental tasks in chemical and materials sciences but also the design and selection of experiments. SDLs combine digital tools and automated hardware to optimize research processes, reduce material usage, and accelerate materials and molecular discovery. This perspective article explores two paradigms for democratizing access to SDLs: centralized facilities and distributed networks. We discuss the technical and collaborative challenges in realizing SDLs' potential to enhance human–machine and human–human collaboration and address grand challenges in science, ultimately fostering a more inclusive research community.

Introduction

In the never-ending arms race between the complexity of world problems and research, the execution and planning of experiments have become increasingly more rigorous and automated. Experimental planning has gradually evolved from random to statistically driven design of experiments; meanwhile experimental tools have advanced from simple facilitators of manual actions to highly automated platforms. As the complexity, intersectionality, and scope of challenges in energy[1], medicine[2,3], ecological harm reduction, and nonrenewable-resource management increase, laboratory research must again leap forward: from individualized research to massively collaborative efforts to incorporate diverse expertise and techniques. In order to bring experimentation into the hands of a broad and diverse community of scientists, however, a certain level of automation, throughput, and accessible design must be achieved.

Autonomous, or self-driving, laboratories (SDLs), are the result of technological efforts to automate the execution of experimental tasks to meet the demands of industry and academia, the design and selection of experiments to minimize the material and temporal costs of research, the refinement and generation of hypotheses to discover new relationships and knowledge, and the collaboration of multiple research groups to accelerate research[4]. An SDL typically comprises a suite of digital tools to make predictions, propose experiments, and update beliefs between experimental campaigns and a suite of automated hardware to carry out experiments in the physical world; these two components then work jointly towards some objective (*e.g.*, process or material property optimization, compounds or property-set discovery, self-improvement, and combinations thereof). The primary differences between established high-throughput/cloud and autonomous laboratories lie in the judicious selection of experiments[5], the adaptation of experimental methods[6], and the development of workflows that can integrate the operation of multiple tools. This automation of experimental design provides the leverage for expert and literature knowledge to *efficiently* tackle the increasingly incomprehensible, multivariate design spaces required by modern problems[7]. *Adaptability* allows for SDLs to develop new techniques to handle new applications, expand the feasible experimental design space, and modify workflows on-the-fly to address and preclude safety and sustainability concerns[8]. Furthermore, the *integration* of tools, learning modules, and data enables SDLs to accumulate knowledge and continually improve.

As a tool for research, SDLs, by acting as highly capable collaborators in the research process, can serve as nexuses for collaboration and inclusion in the sciences by helping coordinate and optimize grand and intersectional research efforts and by reducing the physical and technical obstacles of performing research manually. When combined with collaborators who bring broad domain expertise, this potential new paradigm for research (SDL-assisted research) could allow for the scientific community to adequately address open Grand Challenges[9] which were previously intractable (such as developing economically viable solar power technologies and industrial processes, making breakthroughs in personalized health and safety, and the creation of new analytical devices and methods).

The democratization of SDLs is a necessity to fully realize their promise[10,11]. A team-science research paradigm involves more actors to conduct research and incorporates more diverse ideas into the formulation and execution of research problems. Toward the democratization of research through SDLs, there is an open question as to how SDL technologies will be balanced between open-access, centralized facilities (a Centralized approach)—similar to the European Organization for Nuclear Research (CERN) research facilities and the BioPacific MIP[12]—and networks of distributed facilities (a Distributed approach)—similar to the Galaxy Zoo[13] and Foldit[14] projects and the Harvard Clean Energy Project[15]. SDLs stand poised to address research challenges whose scale and complexity are beyond the limits of comprehension for teams of humans—from molecule and process discovery and optimization to property characterization for specialty applications to kinetic and mechanistic studies. Both the access to scientific research that SDLs provide and the communities that SDLs necessitate and foster position this research paradigm particularly well for enhancing human–machine collaboration, multi-disciplinary and data-driven research, public outreach, and science education[16]. Furthermore, by accelerating research, SDLs involve industry partnerships, whose economic interest in efficient research and development can provide the support to build and improve SDL technologies. These external actors will require the personnel to build and maintain SDLs—which in turn involves more people to engage with the technology and can bring in more industry scientists.

Recent efforts on prototype SDL platforms and their associated technologies demonstrate the first steps of democratizing SDL-assisted research. Numerous systems have been released with open-source tools such as Chemspyd[17], PyLabRobot[18], PerQueue[19], and Jubilee[20] among others[21–28]. Access to such tools facilitates others in developing their own research platforms. Others have demonstrated collaborations between research groups[29,30], across academic levels[31,32], and with industry partners[33] as well as tools which increase accessibility to non-computer scientists[34–36]. Moreover, additional studies have begun characterizing and benchmarking the performance of current SDLs[31,37–39] to facilitate communal comparison and improvement. While these efforts and other SDL technology demonstrations[40–44] inspire hope for the future of SDLs as a democratizing agent in scientific research, there are critical challenges which need to be addressed.

In this perspective, we first discuss two paradigms by which SDLs can be made accessible to the research community: a centralized approach and a distributed approach. In light of these two potential futures, we discuss the current roadblocks towards achieving such a democratized future of SDL-assisted research before addressing how we might overcome these obstacles.

Balancing a Centralized and Distributed Future

While the creation of automated experimental *apparatus* may be feasible for a general laboratory, the effort required to develop and maintain an SDL is unarguably large. To concentrate efforts and personnel into key locations, collaborations have created centralized facilities that allow (virtual) access by application[45–51] (**Figure 1**, left). In an alternative approach, to leverage specialization and modularization towards creating a network of facilities for peer-to-peer collaborations, open-source projects[52,53] have sought to provide general access to autonomous research tools (**Figure 1**, right). As a hybrid approach, simplified, low-cost versions ("frugal twins"[54]) of powerful automation systems can be accessed by individual laboratories for the purpose of development, testing, and troubleshooting before submitting the final workflow to a central facility. Moreover, to tailor capabilities to the needs of specific research groups, individual laboratories could develop a singular instrument in accordance with guidelines from a central facility such that the unit could be temporarily installed in a centralized facility[55].

Centralized, distributed, and hybrid approaches seek to keep SDLs open to researchers regardless of background or financial means and ensure that an enclave of privileged facilities do not have sole access to SDL—a configuration that would not only worsen disparity between laboratories for funding and publication but would also squander the potential of the SDL-led research paradigm. Despite these varied approaches, the challenge remains of *how to ideally balance priorities between advanced, communal automation technologies and networks of specialized platforms*. The optimal strategy for SDL deployment must consider how the initial investments (the barriers to entry) are overcome, how logistics and legal concerns are managed, and how the workforce is prepared to engage with SDLs in industry and academia.

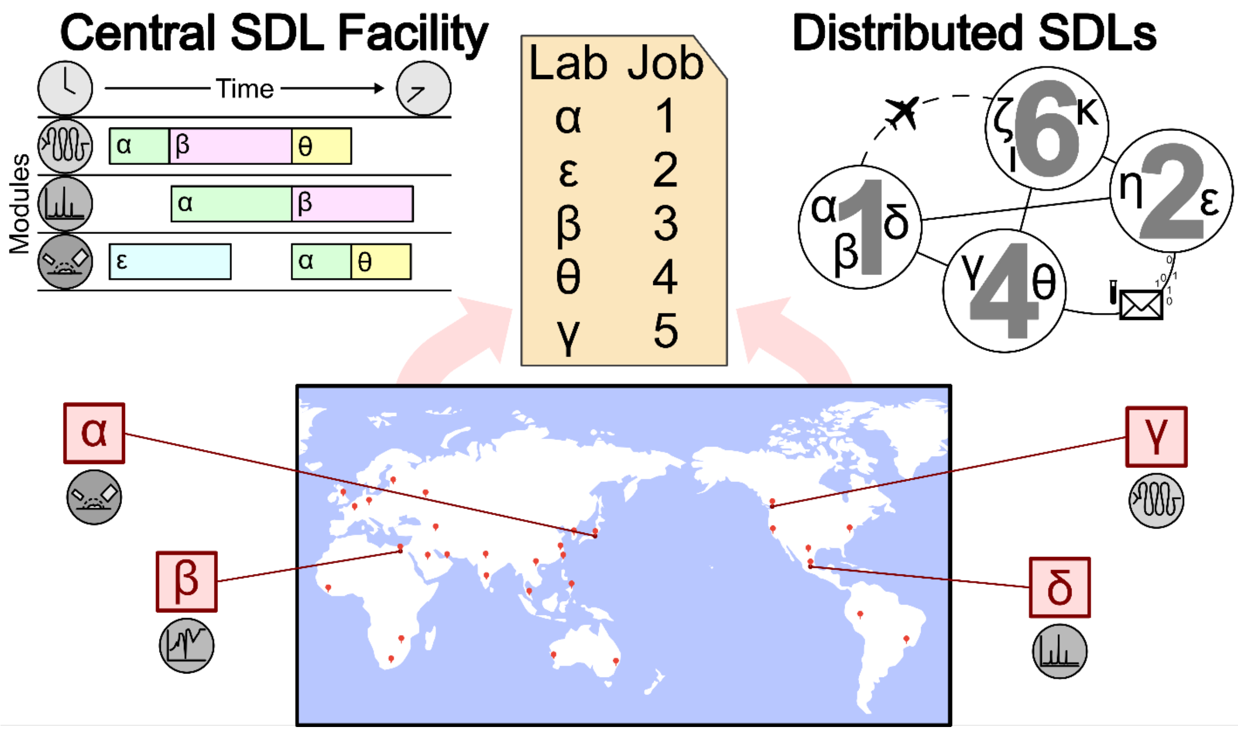

Figure 1. *Schematic illustrating both centralized (top left) and distributed (top right) SDLs. Laboratories are represented with Greek letters, their requested jobs with numbers, and capabilities with icons in gray circles. In the centralized approach, multiple laboratories submit their requests, and time on various center facilities are equitably distributed between modules throughout the day. In the distributed approach, various (temporary) groups form around complementary capabilities and the groups can distribute tasks amongst themselves, share information, and transmit instructions and materials as appropriate.*

In terms of financing and staffing, centralized facilities may be more attractive to industry investors and national funding agencies, as funding a single meta-project helps guard against splintering and wasted/redundant effort, helps maintain long-term collaboration, and provides more stability (less risk) than an individual research group[56]. As the costs of commercial automation units and software decline, distributed SDLs become more feasible. Smaller, designer SDLs are in turn likely to attract local businesses and universities. The proximity and flexibility of distributed SDLs can facilitate rapid collaboration on novel and cutting-edge research for a given scientific or industrial niche—provided the rest of the SDL technologies are already in place (or the collaborator can tolerate the investment). Conversely, a centralized facility may have too much inertia to rapidly address changing needs or may struggle to justify providing highly specialized equipment that only a handful of users ever use.

The maintenance and sustainability of the SDL ecosystem is also dependent on good management. Team-science management, regardless of approach, requires the coordination of data and experiments in a manner that is both robust and equitable[57,58]. The distributed approach, with its more liquid boundaries, would require significantly more coordination, making maintaining the digital aspect (digital twins and datasets) more difficult[59]. The centralized approach raises ethical questions of how projects are selected, time and resources allocated, and experiments managed. Both approaches, in different ways, also raise ethical questions about the proper attribution of credit, the costs of material, and the sharing of materials between projects when research is conducted outside its parent laboratory. Beyond these issues of self-regulation, there are also external regulations which must be considered.

In democratized science, data must be generated safely, ethically, and legally and the quality of the data must be made trustworthy[60]. With respect to local and national regulations for hazardous materials, dangerous processes, and sensitive data, it is not clear which approach, centralized or distributed, is a better fit for the near future of SDLs. A centralized facility may have an easier time being regulation certified, but also must acquire more or higher-grade certifications; whereas a smaller SDL in a distributed network can only apply for the certifications it needs but may struggle to acquire all the engineering controls required to meet the certification. Concerning data quality, any SDL would require routine testing and quality control in order to maintain public trust in addition to study-specific benchmarking and control experiments to ensure the validity of results for new or novel materials and processes. In the centralized approach, a consortium of key facilities could develop these protocols and use them as the standard; whereas in the distributed approach, significantly more effort would be required to create robust future- and site-proof standards for interoperability, shareability, and reproducibility with periodic checkups to remain a trusted member of the network of collaborators. While overall maintenance and standardization may be easier for centralized facilities, it is worth noting that it is likely that the research groups using these facilities may find the established protocols and standards limiting in what research can be conducted.

SDLs must engage with and support their collaborators: *people*.[29] Any proposed education strategy implemented should reinforce itself to ensure the sustainability of the SDL ecosystem. By participating in an autocatalytic cycle of training future users who can improve SDL systems and better communicate with others, these future experts are more able to train the next generation of scientists and industrial users who can in turn further improve SDLs. In the centralized paradigm, key facilities create centers of learning where experts can gather and share wisdoms. These facilities can then act as educational institutions that can provide intense and fulfilling education for participants. Conversely, in the distributed paradigm, having more diffuse facilities can more effectively provide access to a geographically diverse cohort of future SDL researchers and may have a larger overall capacity—increasing the number and diversity of future-researchers benefited. Furthermore, low-cost and do-it-yourself SDL technologies can serve as educational tools for burgeoning researchers (*e.g.*, "frugal twin" platforms[54], Educational ARES[61,62], and Legolas[63]). Ultimately, the democratization and use of SDLs is in service of people, and how users are trained in and engage with these powerful research tools must be thoughtfully considered.

In both paradigms, the goals to increase throughput or reduce cost must be balanced against the quality of the data (**Figure 2**). Experimental fidelity can greatly impact the number of experiments required to arrive at a solution[39,64], and further work is required to determine the optimal tradeoffs between these design goals. Any low-cost system would need rigorous reproducibility analysis to be of value to SDL-aided research. The relationship between setup and operating costs and data fidelity will evolve with the advancement of automated laboratory technologies and in turn modify the optimal balance between centralized and distributed SDL research. The democratization of SDLs is a continuous process and will necessitate and support both an increase of team-science and the advancement of accessible, automated laboratory technologies.

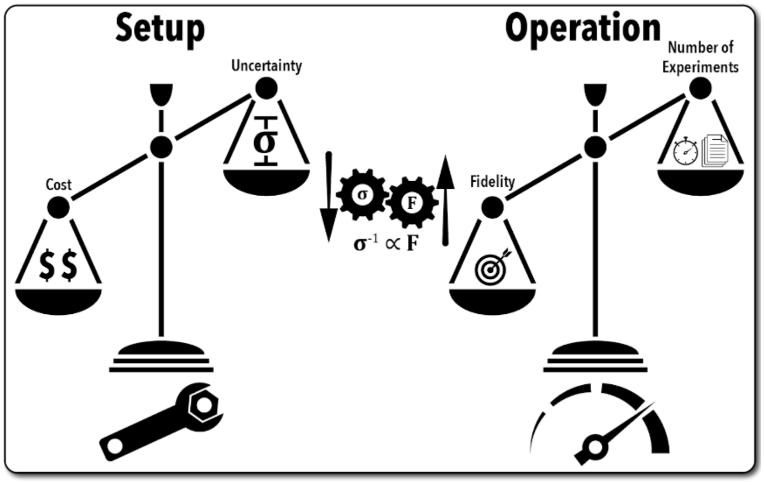

Figure 2. Illustration of the tradeoff between initial investments improving experimental fidelity and the number of experiments (thus operating costs) required to achieve a goal on an SDL.

Roadblocks on the Path to Future SDLs

SDLs have the potential to expand (or restrict, if improperly managed) who is afforded the opportunity to do research. There are significant hurdles which hold back SDL technologies and forestall their democratization (**Figure 3**). Individual SDLs are large projects, and current demonstrations of SDLs are limited by hardware and software capabilities or are deployed conservatively to reduce risk. As a result, there are few exemplar systems that are industrially relevant enough to attract widespread funding, and funding is required for high-impact demonstrations. Support from outside this cycle is needed to kickstart SDL proliferation, and efforts made to democratize both physical and digital aspects of SDLs are necessary.

In this section, we review the major roadblocks to SDL proliferation and to the subsequent democratization of automated research technologies. The discussion will focus initially on the digital aspects and physical aspects of SDLs, then the generality of SDLs platforms and matters of user trust and workforce development, then finally on the challenges of attracting non-academic support for the technology.

Machine Learning and Autonomy

The integration and automation of advanced data-science strategies for the analysis of results and the proposition of new experiments is a key feature which separates SDLs from prior work in high-throughput experimentation. Currently, machine learning (ML) for materials and molecular discovery is primarily used as a virtual screen for candidate samples (simulating experiments, *i.e.*, sample to property) and as an experimental planner (simulating rational design, *i.e.*, property to sample). Virtual screens can be applied iteratively, with increasing fidelity (and computational cost) at each iteration to efficiently move from a large candidate space to a manageable set of promising candidates for experimental validation. Synthesizability is often one of the last virtual screens to be performed, despite its necessity and restrictiveness, due to its computational cost—a challenge which has motivated incorporating synthesizability into experimental planning models[65–68].

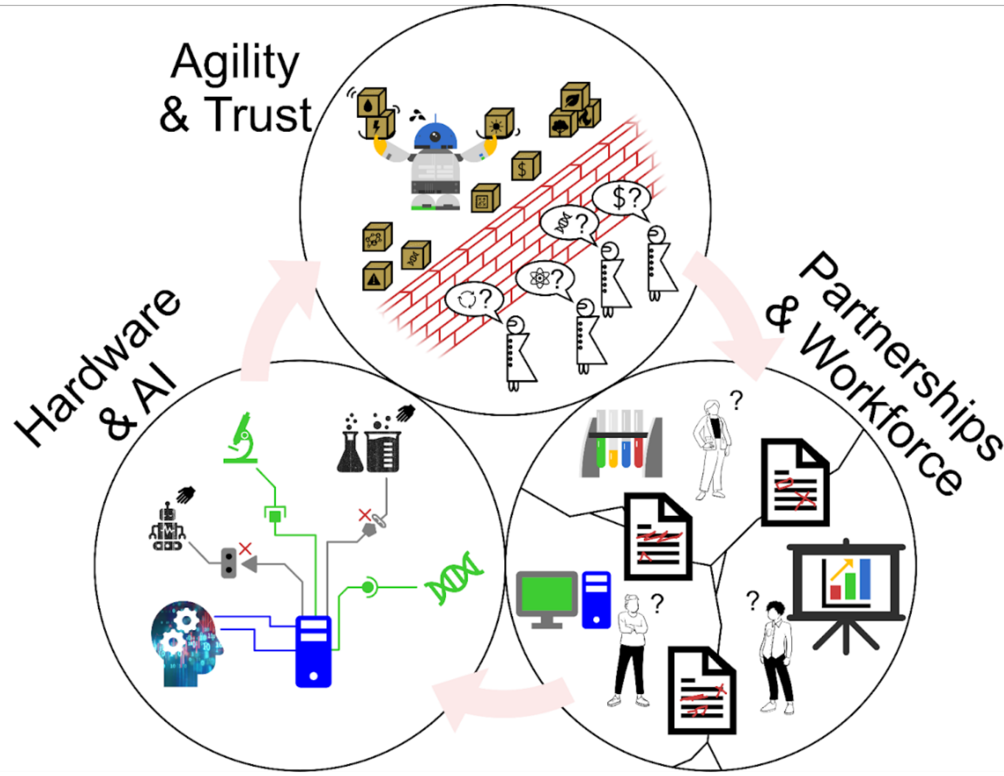

Figure 3. *The cycle of challenges forestalling the advancement of SDL technologies. Incomplete integration of AI, hardware, and software prevents the creation of agile experimental systems and the complexity of these systems renders SDLs into black-box systems which can struggle to balance all the requests and questions given to them. Questions and requests to different aspects of SDLs receive unclear answers and this incomplete information results in difficulties collaborating with other scientists and industry partners, which in turn impacts funding and support. A lack of cohesive support challenges the advancement of human–AI–robotic collaboration and the improvement of SDL technologies, starting the cycle anew.*

The development of multi-objective ML algorithms for automated experiment suggestion is typically not as trivial as running multiple single-objective algorithms simultaneously. Single- and dual-objective workflows have demonstrated great potential[69], and have enabled both closed-loop (no human intervention—often excluding restocking or maintenance)[3,70,71] and hybrid workflows (*e.g.*, electron and scanning probe microscopy[23,26], synchrotron scattering[72], *etc.*). These successful demonstrations have required two important prerequisites for the ML component: well-defined cost/feasibility constraints and a robust reward structure. Constraints can often be specified using prior knowledge about the experimental system or be learned during experimentation. The reward structure, however, presents compounding challenges for multi-objective and future-looking ML algorithms.

One concern for multi-objective rewards is that in physical systems, the property–structure spaces are rarely smooth (*sc.*, a core assumption of many ML models).[73] While algorithms to handle non-smooth property-structure spaces are in development[74–76], their translation to experimental systems remains a work in progress. Another concern for multi-objective rewards is that physical and chemical properties are often correlated, and so a naive composition of rewards from individual models may overfocus on a subset of properties[77]. Material or molecular synthesis and purification can take hours to complete, yet some characterizations can take seconds (*e.g.*, spectra) to years (*e.g.*, ambient stability). As a result, model components must either become desynced or propose multiple rounds of experiments before receiving feedback[70]. Finally, there are some objectives which are difficult to express mathematically or provide immediate feedback to the model. For example, future-seeking objectives such as "optimize for sustainability" or "discover a greener pathway to a chemical product" need to be translated into short-term measurables (*e.g.*, toxicity scores, material use, stability, waste generation, supply chain carbon footprint, monetary cost, *etc.*). Each short-term measurable comes with its own set of questions (*e.g.*, metric/assay choice, comparison techniques, economic contexts, *etc.*). New ways of combining and translating objectives[78–80] are required to address complex or unclear connections between objectives (low- and high-level, immediate and far-off).

To address the latency concern, the use of digital twins[81] or proxy measurements[82] has been proposed. A digital twin is a rigorous model of the experimental system which can be used to provide simulated results until the true results are obtained (as well as help with screening proposed experiments). This approach can address disparate timelines for feedback but will slowly fall out of touch with reality. Proxy measurement is the estimation of a difficult or slow to measure property of interest by using correlations to a property that is quick or easy to measure—necessarily requiring finding such a pair (or set) of properties and developing the correlations[83]. Proxy measurements can struggle in material discovery (extrapolative) campaigns and so require continually maintaining the correlations with new data. While these approaches address latency, they bring uncertainties as to how to connect these models/proxy measurements back to long-term goals as they replace real measurements with model predictions or correlations.

A final, foundational ML challenge for SDLs is understanding and quantifying uncertainties. The uncertainty of the experimental proposition model and the property prediction models (as well as the value of specific results relative to the total objective) are crucial for determining which experiments are proposed. These uncertainties provide a crucial touchstone for human collaborators as a rough estimate of how confident[84] the ML algorithms are. These uncertainties can be estimated using ensembles of models[85] and can be augmented by experimental uncertainties of the SDL[86]. Current SDL hardware can make capturing some experimental meta-data challenging; and despite manufacturer testing, experimental uncertainties must be measured for the particular chemical or material system being investigated. Armed with this information, however, an SDL may be able to improve its own workflows for material discovery and process optimization—learning about both the experimental topic and laboratory praxis. Less speculatively, uncertainty, calibration, and benchmark studies are required for human researchers and collaborating SDLs to determine their trust in SDL-generated results. Despite how crucial such studies are, the current suite of tests and the integration of these controls into SDL workflows is lacking. Without these tests, SDLs are not able to fully participate in science.

Laboratory Automation Technologies

Laboratory automation is a powerful tool and bridges the digital and physical worlds of SDLs, enabling active learning. Over the past few years, there has been a rapid growth of laboratory automation in research groups, ranging from (partially) automated facilities such as Emerald Cloud Labs[45] to academic research systems[48]. To date, proof-of-concept automated setups have been demonstrated for many steps in the traditional materials science research workflow, including precursor formulation[87], solid-state synthesis[88], materials processing (such as printing[31] and thin-film deposition[89]), isolation[3,90,91], and characterization[92]. Moreover, robotics solutions for sample transport have improved the accessibility and capabilities of both flow- and batch-based systems. The integration of disparate components into a single, usable platform (even in a modular fashion) requires establishing engineering controls, networking systems, defining a data-collection and management structure, and providing human access points for troubleshooting and collaboration.

Developing automation tools and integrating them into SDLs relies heavily on access to application programming interfaces (APIs) and the documentation of both these APIs and the tools' capabilities[82]. Few APIs are readily provided by manufacturers and many are poorly documented or come with restrictive licensing agreements. Combined with limited vendor technical support, the burden of developing APIs often falls on researchers—reduplicating efforts between groups and producing solutions which are not universal. The success of platforms like Opentrons[20,93–97], which despite its relatively simple capabilities and intended use as a biologics platform, underscores the importance of open-access systems and accessible APIs in fostering innovation and adoption in SDLs. The rise of open-access, low-cost systems, such as the Chemputer[98], Molecule Maker[51], Jubilee[99], and others[100,101], further highlights that the openness and reconfigurability of automation platforms are significant factors in their adoption.

As an emerging field, off-the-shelf hardware has often focused on general-purpose use and high-throughputs—the latter of which is necessary to make SDLs effective research tools. Chemical and materials science, however, imposes heavy demands on system robustness, and the dynamic, specialized needs of cutting-edge research require flexibility not currently available in commercial units. Despite the falling cost of many individual laboratory hardware and software solutions, the escalating complexity and breadth of SDLs has prevented their proliferation—particularly in academic and start-up environments where financial allocations can fail to keep pace with inflation and the time-to-deliverables is constrained. Research laboratories and commercial manufacturers must engage in a market- and science-driven dialogue about SDL technologies: should a manufacturer wish to capitalize on being part of the SDL ecosystem, it must provide and support programmatic access to its products. A commercial manufacturer is likely, however, to include this integration as an *a-la-carte* service—adding another cost. While it is possible to forgo putting APIs behind a paywall, as the prior Opentrons example exemplifies, the commercial supplier would be betting that increased hardware sales would make up for the lack of API sales.

Due to the size of the research market, vendors may not foresee sufficient economic returns in recapitalizing their product lines, especially when contrasted with closed ecosystem approaches that are potentially more profitable. Moreover, vendors may be averse to open-source systems that are interchangeable between vendors for similar potential-profit–based arguments. These financial motivations inhibit integrations between vendors and, in turn, the rapid adoption and advancement of SDL solutions. Consequently, individual research groups are developing their own systems for their own specialized needs; meanwhile, most groups, especially in industry, would rather purchase a working off-the-shelf SDL.

Further compounding the economic barriers to SDL development, research funds are mostly allocated towards scientific results, rather than the infrastructure and development needed for SDLs. The current research funding ecosystem results in bootstrapping and leveraging of funds to build SDLs. In addition, the singular focus on the scientific results of interest can result in hardware and software which are tailored to (or even pigeonholed in) a specific application—reducing the generalizability of SDLs. Furthermore, student theses are harder to award for tool development than for scientific advances, relegating SDL development to the leadup to the published work. Therefore, it will be important that investments be made in SDL infrastructure, with the understanding and expectation that these new tools will lead to new and impactful scientific advances.

Looking ahead, we anticipate exciting breakthroughs that will expand the capabilities and diversity of lab automation technologies. A growing number of case studies[102] demonstrate that collaborative workflows, where human and robotic systems work together, can achieve synergistic benefits. Incorporating humans into complex experimental workflows is not necessarily a transitional step toward full automation; it can be a tailored approach that maximizes system flexibility and efficiency. Moreover, while current state-of-the-art laboratory automation technologies aim to replace human-centric experimental workflows with robotic maneuvers, the next generation of laboratory robots is expected to possess the capability to create new workflows. These will leverage the geometry, precision, and complexity of mechanical hardware and make timely decisions using ML, rather than merely replicating how humans perform scientific tasks.

Automatability and Agility

Despite open-access efforts to facilitate the sharing of SDL technologies, their transferability in practice can be limited. Control and data systems need improvement to address the dilemma between the desire for generality (being applicable to any hardware system) and specificity (taking full advantage of the nuances and capabilities of a given instrument)[103].

While the accessibility and power of APIs has been discussed in the previous section, vendor-provided APIs may transmit data in proprietary or otherwise opaque data formats—complicating the data analysis required for self-driving operation. Academic[18], commercial[104], and governmental[105] research efforts into providing open-source and simplified APIs and SDL development tools show promise in making SDLs more accessible and interoperable. These open-source and more homogeneous interfaces (*cf.* bespoke interfaces) have an additional potential synergy with automatic hardware integration and exchange tools enabled by LLMs (*vidē īnfrā*).

Many members of the SDL research community (and some journals[106]) have actively embraced the public release of data and code as part of the publication process. This open-source strategy benefits even groups which must develop their own "home-built" solutions (for legal, competitiveness, or technological novelty reasons) as the open-source libraries can be referenced and components can be reused—provided sufficiently modular design. This push for the open-sourcing of published software must be only a starting point. Successful open-source packages require long-term software engineering and maintenance, which are incompatible with typical academic research funding mechanisms[107]. The popular open-source libraries for ML development are largely maintained by the technology industry. For SDL software, however, releasing a package as open-source then hoping that "the community" will take care of it is overly optimistic. Complicating cyber infrastructure needs, the threat of open-source tools being used to hack SDL systems poses real-world physical safety and intellectual property (IP) concerns. As demonstrated by the recent XZ Utils incident, open-source software is not impervious to malicious actors[108]. Security will become a major concern as SDLs amass more data and centralized facilities become prime targets for data-theft and denial-of-service attacks.

Data-management and modeling must be flexible, interoperable, and provide representations of experiments and results.[109] Whereas the motivations and challenges of FAIR scientific data have been discussed elsewhere[110], attempts have been made to organize experimental information in general purpose relational schema[111] and in semantic knowledge graphs[27,112] as well as efforts to provide provenance tracking[113]—a feature which, once mature, will be indispensable for combating dubious data and for general data-management in a distributed paradigm.

ML modules, as well as virtual experiments, also require automation. There has been a growth in the development of software packages that automate the creation, training, fine-tuning, and deployment of ML algorithms for a variety of contexts (*e.g.*, ChemProp[114] automates the creation and deployment of ML models for molecular property prediction). Considering the ubiquity of optimization as a problem, numerous software packages have emerged for single and multi-objective optimizations in general (*e.g.*, Ax[115], Dragonfly[116], gpCam[117], scikit-learn[118], *etc.*) and in chemical and materials applications (*e.g.*, Olympus[119]). Despite their utility and demonstrated power, the incorporation of appropriate domain knowledge (*i.e.*, constraints and compositional-/permutational- invariances of the search space)[120] is still encoded manually by expert users.

A complete workflow must combine instrument control, data-management, and experiment planning together, performing an iterative cycle until the specified goals or other stopping conditions have been reached. These types of workflow management software tools are well-developed for computational research, but comparatively nascent for SDLs. Examples of SDL workflow managers include ARES OS 2.0[121], Atinary[122,123], ChemOS 2.0[124], NIMS OS[125], and BlueSky[104], in which the general process (experiment types to be performed, types of optimizations to be conducted, stopping goals, *etc.*) are programmatically defined. Distributing experimental workflows across multiple geospatially separated sites is a long-standing interest in this field, and methods adapted from computational workflow management have been applied to this problem.[70,126]

A long-term goal of SDLs is for them to have the ability to freely generate workflows toward high-level goals. Several groups have recently demonstrated higher-level artificial intelligence (AI) agents using pre-trained LLMs to elicit a goal from the user in natural language and then iteratively taking actions by calling external “tool” programs (which perform physical operations, measurements, simulations, and literature searches, *etc.*).[35,127–129] Existing LLMs are best understood as approximate search and retrieval engines that mimic the planning present in training examples, and their unpredictability requires special attention be put into engineering operational safeguards[130]. In addition, the current best ML models for laboratory automation are commercial products and lack public information about their training data, reproducibility or consistency metrics, hallucination rates, and precise methods—traits which render them undesirable for scholarly purposes. For the near term, achieving genuine planning with LLMs requires considerable supplementation with more traditional, logic-based verification workflows[131].

LLMs present an opportunity to automate the translation and integration (interoperability and efficient communication) between different robotic systems. Presently, a considerable amount of time and resources is spent on manually developing "glue" software to facilitate interaction among disparate systems. While powerful middleware, protocol, and orchestration tools such as ROS[132], SiLA 2[133], and BlueSky[104] that aim to address these interoperability issues have been developed, their adoption is limited to groups developing the most complex SDLs, pointing to a broader issue of fragmented technology ecosystems within laboratories. These middleware suites have learning curves that can challenge less experienced groups and are sufficiently abstract (due to their universal design) that they can be difficult to quickly deploy for a specific application. Conversely, for the larger projects of more experienced groups, version management and overhead can become a concern when using these frameworks[134] and may motivate a group to create its own middleware suite. Consequently, the progress by less experienced groups is limited by their lack of awareness or expertise in the technology and progress by more experienced groups is not easily transferable to other groups.

Transparency and Trust

As a consequence of experimental planning, execution, and analysis being automated (especially when done so in an *ad hoc* manner), there have been concerns about whether the data generated by an SDL can be trusted. While *ad hoc* solutions are indispensable during the early stages of a technology's development, they often result in increased setup times and suboptimal outcomes as many laboratories "reinvent the wheel"[18,135,136] or implement methods developed by non-experts. This makeshift approach not only delays the operational readiness of SDLs but also introduces the potential for unreliable experiments. Ultimately, the need for trustworthy data is two-fold: accurate, precise, and reproducible results are foundational to the scientific method and any democratic use of SDL technologies is susceptible to being poisoned by bad data[39,64]. A democratized SDL future will involve immense data sharing and the quality of this data is paramount to ensuring efficient experimentation, practically useful results, and safe operation. When deployed properly, SDLs could be used to automate the verification of claims made in the literature[137].

Cross-validation establishes and quantifies trust. It is important, then, for existing platforms to participate in validation studies in order to resolve irreproducibility issues, help industry quantify the risks of investing in SDL technologies, and supply training data for endeavors in mapping operations between different hardware architectures—ultimately accelerating collaboration by improving the transferability and interoperability of SDL technologies and experimental results. Many extant SDLs, however, are beholden to their externally-funded project's goals (particularly in academia) and either do not have the bandwidth to repeat others' studies or conceal crucial aspects of their workflows to protect their sponsors' IP (curtailing the cross-validation of their results by other SDLs).

At present, most laboratories can only report calibration, benchmarking, and self-validation data to garner support—with only a fraction of SDLs actually incorporating repeated validation experiments to mitigate systematic errors or reporting repeatability metrics for benchmark experiments. There are, however, no standards for performing or enforcing such studies and incentives are non-existent. Different fields and applications have different ideas of what is considered standard for experimental verification; and for multidisciplinary and multi-application SDLs, these discrepancies make defining a singular standard difficult. For example, SDLs must often justify the abridgement[3] of otherwise ubiquitous characterizations of nuclear magnetic resonance and mass spectroscopy or x-ray diffraction due to the mismatch in throughputs (particularly with the workup for the characterizations).

For distributed SDLs, the completeness and thoroughness of platform and results characterization (meta-characterization) must be studied such that collaborators can properly assess literature data. Centralized SDLs may be able to create *de facto* meta-characterization standards through their internal policies and the requests of users. As hardware advances, however, it becomes necessary to standardize how mechanical components of SDLs are specified[138] and to train personnel in their proper maintenance. Generally, duplication of research and development efforts for SDL equipment should be reduced to only what is necessary for cross-validation. Similarly, as data formats and software evolve, best practices and standards change, and the preferred programming languages for scientist-programmers shift in popularity, the code- and data-bases of an SDL must be properly maintained and tested in order to avoid bit-rot[139]. The protocols for communicating with centralized facilities or between distributed SDLs are probably the most susceptible to changes and frequent maintenance as they are directly tied to larger internet infrastructure, cybersecurity, and evolving research objectives. Until either a critical mass of SDLs is online or the self-reporting of platform metrics is sufficient to assuage investment risks, the lack of trust to justify SDL-investment will remain and the growth of SDL technologies will be stymied.

Simultaneously, the adoption of comprehensive data collection and analysis remains inconsistent. For SDL technologies to thrive, data must encompass not only experimental results (inputs and outputs) but state and environmental information as well (*e.g.*, temperature, relative humidity, and any metadata required to reproduce the results of the ML models—measurables often overlooked by commercial units)[60,140,141]. Within a domain (*e.g.*, organic chemistry, materials science, biochemistry, *etc*.), there can be multiple representations for the same material; for SDLs at the intersection of multiple domains (and modalities, *i.e.*, experimentation vs. simulation), this challenge of representation is only exacerbated. For SDLs to be effective, it is not enough that data be accessible over the internet, data must be readily usable (machine-readable), transferable across domains, and have associated confidence levels to let researchers (and SDLs) make informed decisions about using them. While epistemological and ontological frameworks are in development[27,142] and can facilitate collaboration across linguistic, domanial, and cultural barriers, they represent yet another complex system which must be integrated into an SDL. The development and maturation of a standard formalization of data collection and sharing for SDLs will take time; yet there is an opportunity for a near-term solution in using LLMs to aid in translating between different research groups' and commercial units' data-management formats.

Workforce Development

The transition from conventional to autonomous research in the materials and chemical space will require developing a specialized workforce that is multi-faceted and fluent in a number of disciplines. The *status quo* of research favors collaborations between others in a similar field (such as chemical engineering and materials science, or robotics and computer science) or between members of the same research campus. Unfortunately, the applications where SDLs are most promising also require the greatest mass of knowledge. The interpretation of results is further complicated by the throughput and potential depth of data which an SDL can generate[143,144].

The needed workforce is not, however, a monolithic body: the skills needed to realize, use, and maintain the autonomous research enterprise are not the same. To respect this granularity, we propose to consider the workforce development challenges and opportunities in terms of three classes of participants (**Figure 4**). In particular, we consider *developers* that combine hardware, software, processing, and materials innovations to realize new autonomous systems; *technicians* who are responsible for maintaining and tuning such systems; and *users* who primarily interact with autonomous research systems through the digital world by selecting hypotheses, guiding learning, and analyzing data. While these may be distinct roles, it is important to acknowledge that individuals may move between these roles throughout the course of their career and as their research needs evolve. Moreover, these roles will require differing levels of expertise within and between fields as well as collaboration skills. As complex engineered systems that lie at the intersection of multiple domains, SDLs will need a healthy distribution of actors to be successful.

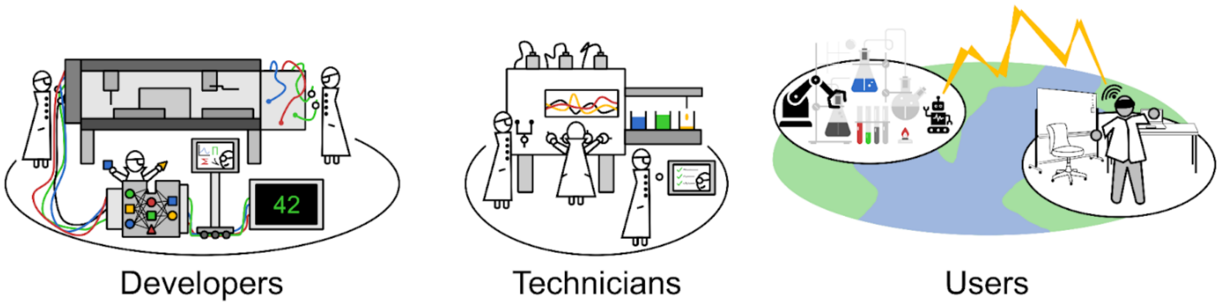

Figure 4. *Schematic of the three primary roles of SDL personnel: developers, technicians, and users.*

The developers of autonomous experimentation systems must combine the dual expertises associated with their experimental domain and automation. They must know the subtleties and pitfalls of various laboratory and research techniques in their discipline and be skilled in robotics and software control to provide programmatic control which aligns with their nuanced scientific understanding of the process. In contrast, traditional academic departments are fairly siloed with robotics being separate from chemistry or materials science; and learning to be a developer generally requires dedicated training and learning to fill the educational gaps as well as practice. The need for practice systems can be ameliorated with low-cost systems that have been specifically designed as pedagogical tools.[63,101,145,146] The development and dissemination of such systems is an important part of efficiently training SDL developers.

The challenges associated with maintaining SDLs mirror the challenges in developing them. A technician may be required to monitor processing signals to ensure smooth operation, intervene to repair or recalibrate the system when needed, and restock supplies. Technicians are not required to have the depth of expertise in the underlying science or robotics optimization as would be required for developers. As such, individuals with some experience with physical experiments, whether vocational or through undergraduate training, and instrument-specific training will be able to perform this role. Here, micro-certifications and online training (offered by an academic institution or manufacturer) are appropriate for delivering the specific knowledge needed to operate the relevant systems. Both the academy and industry should be involved in the development of these resources.

A fascinating opportunity enabled by SDLs is the opportunity for researchers to interact with them in a purely digital sense. Whether decentralized or centralized, future SDLs may connect to users from distal institutions. The user's two main responsibilities are to (1) formulate good scientific hypotheses for the SDLs to explore and (2) oversee the learning process to make adjustments as needed. While the former can be thought of as a goal of doctoral education (implying most first-generation users will be domain experts), in contrast to a developer, this domain expertise could be purely computational. For proficiency in the latter task, users will have to practice overseeing the SDL. Facile tools that allow for this experience and pedagogical resources that define the types of situations that can be experienced (and how to resolve them) are needed[147].

While the collaboration between industry and academia is necessary for the advancement of SDL technologies, there is a conflicting argument between what each group seeks to gain from the advancement. A *user* seeking to apply the SDL to solve a scientific problem or perform a rote action may desire a more vertically integrated SDL technology, which packages hardware control, data-management, and experimental planning together (such as Atinary[122] or a lab-as-a-service provider such as Emerald Cloud Lab[45], Frontage Lab[148], Certified Laboratories[149], *etc.*). A *developer* seeking to advance laboratory capabilities may desire the ability to combine, adapt, and create new modules—favoring horizontal integration. A party more interested in workforce development, education, or mitigating job displacement[150,151] may desire to have components developed and implemented in-house as a form of training. These cases must be balanced so as to provide the equitable advancement of the technology (theoretical and demonstrated) and the workforce.

Successful efforts in a collaborative SDL will require *team science*[152] to communicate with diverse researchers and people who may not have shared research experience, vocabulary, or knowledge base—a cultural exchange applying to both new students and seasoned experts alike. Large, disparate teams are more vulnerable to failure because of the lack of shared knowledge, and shared goals. These teams will need people skilled in team science who can facilitate development and success of the team—a role currently not prepared by academia. There are some programs such as the "Growing convergence research" program at the National Science Foundation (NSF)[153] that are pushing this area. A consequence of this lack of a teaching culture is that teamwork is most often learned "on the job". While it is not possible to master team science wholly within a degree program and this skill is a lifelong learning objective; it has yet to be determined how this skill set should best be integrated into educational programs.

Finally, there is the open question over how training should be distributed between academic and industrial settings as well as the design of curricula and programs—items which depend on the nature of how the centralized and distributed paradigms are balanced in the future.

SDL Partnership Efforts

Industrial adoption and implementation of SDL technologies are currently limited to a few specific areas, such as biotech, biopharma, and specialty chemicals/materials where companies have applied SDLs in their discovery pipeline[154–157]. While examples have recently emerged in related fields, further de-risking of the technology is needed for a broad market penetration.

Industry-led partnerships bring more than financial resources, they offer access to experts, real-world applications, and commercialization channels. For instance, the IBM–Pfizer collaboration on AI for drug discovery demonstrates how industry support can advance SDL capabilities by combining computational power with pharmaceutical expertise[158]. Unlike purely governmentally funded projects, which are often delimited by specific research outcomes and timelines, industry partnerships can be more flexible. Partnering with academic institutions can provide valuable assets such as innovative research, specialized domain knowledge, and access to state-of-the-art SDL facilities. A compelling offer to industry partners could include tailored research projects that leverage academic insights to solve industry-specific problems, as seen in the partnership between Google DeepMind and various UK universities, where AI research is applied to challenges in healthcare, energy efficiency, and other areas[159]. While traditional funding bodies are typically limited in terms of budget and scope of SDL projects research initiatives (making it difficult to fund ambitious, large-scale projects needed for breakthrough demonstrations), industry participation, can be instrumental in the development of large-scale SDL initiatives—such as the Materials Innovation Factory[160] among others[161–163].

Thorough cost-benefit and other techno-economic analyses are typically required to illustrate the potential savings in time and resources that SDLs offer over traditional research and development processes (*e.g.*, such as high-throughput screening and experimentation) and will help collaborators make the best choice of tool for the challenge at hand. Mature approaches are often viewed as safer investments for addressing new, complex problems, and as SDL technologies advance the question of whether to (or the temptation to) use brute force, high-throughput experimentation will remain as advances in one often apply to the other. While transparent analyses of SDLs may help partners overcome their own barriers of viability, security, IP, and competitiveness, external factors such as legislation over whether compounds or processes discovered by SDLs are patentable hover over industry support.

The fourth industrial revolution (Industry 4.0) encapsulates the profound transformation in industry catalyzed by automation and autonomy[164]. Across various regions globally, particularly in Europe and Asia, many countries are actively embracing and gearing up their economies for this revolution[165–168]. While we remain in the nascent stages of this revolution, the utilization of ML and generative AI in industrial contexts is rapidly gaining traction[169]. The advantages of employing autonomous workflows in industry are readily apparent: enhanced productivity, heightened efficiency in production and discovery, and improved reproducibility and quality control. However, realizing these benefits necessitates overcoming numerous challenges to prepare industries for such a transformative shift.

To support burgeoning industries, it is imperative to fathom the intricacies of developing ecosystems tailored to handle autonomous workflows. The escalating connectivity of data via cloud resources and the Internet of Things necessitates data ecosystems capable of autonomously processing, storing, and harnessing the exponentially increasing deluge of data in a flexible, secure, and sustainable manner. Such data ecosystems have garnered interest from industry, as evidenced by the initiatives mentioned above, as well as from government researchers, exemplified by the recent US Department of Energy blueprinting activity for an Integrated Research Infrastructure[170] and NSF's National Artificial Intelligence Research Resource Pilot[171]. At the Interconnected Science Ecosystem at Oak Ridge National Laboratory, for instance, "architects" are crafting a systems-of-systems architecture and microservices to comprehend the deployment of autonomous workflows across a myriad of scientific domains, including those concentrated on industrial settings like scalable autonomous material development, electric grid emulation/optimization, additive manufacturing, radioisotope production facilities, and agricultural facilities[172].

Collaboration with national laboratories provides a unique opportunity to explore how different lab and academic efforts can be coordinated on a larger scale and provides a testbed for how various centralized and distributed technologies can be implemented. The intermediate scales and technology readiness levels of national laboratory projects, may be optimal for the development of autonomous systems to manage both academically and industrially relevant data provenance and metadata—a challenge that transcends fields and informs how disparate industrial sectors must adapt to embrace autonomous workflows. Whereas a centralized facility can achieve high throughputs through advanced scheduling optimizations and by scaling up, a network of SDLs can achieve high throughputs by numbering up (distributing, and thus parallelizing the workload). If a workflow requires specialized equipment, it is dependent on a central or member facility possessing such equipment. A potential solution is one being explored by BlueSky[104] and Argonne National Labs's[173] SDL facilities whereby the host facility shares its integration standards such that research groups can submit and "plug in" their own devices to handle niche cases. While this requires financial and logistic support for transporting, troubleshooting, and integrating bespoke equipment, it does address the throughput concerns of a single, small facility and the specialization concerns of a centralized facility.

Calls to Action

In our collective advancement toward a more democratized future of SDL-aided research, we must focus our efforts. Depending on the application, different aspects of SDL workflows are identified as the limiting step: for some, SDLs are limited by throughput (synthesis, workup, isolation, purification, characterization, or model-retraining), for others, SDLs are limited by underperforming models, and for others still, SDLs are limited by data collection and management (**Figure 5**). At the core of these issues is the idea that for many SDLs the material and data throughputs between unit operations are mismatched given extant technologies. While advancements to improve individual components must be made, this conflict hints that additional work is needed in the prediction and management of scopes and throughputs when an SDL is being designed[174]. In this spirit, some effort should be made into automating the act of automation by creating SDL "installation wizards" which can help in selecting equipment and developing variations of traditional workflows to make the most of the resources available. Such analysis can also help identify which bottlenecks are the result of funds and which are the result of some fundamental limitation of the technology or technique. The latter invites innovation and can better illuminate the cross-SDL benefit of addressing these limitations—catalyzing the development of new SDLs.

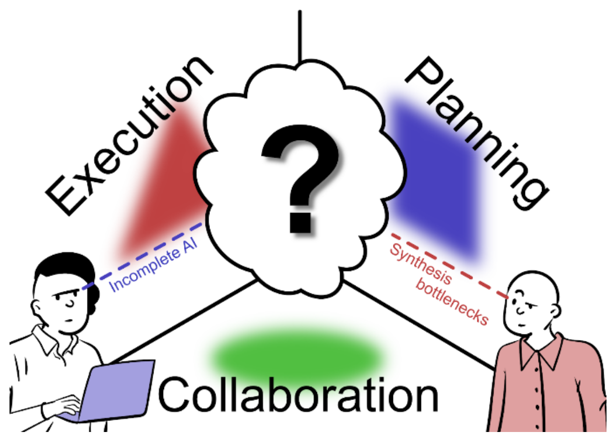

Figure 5. *The challenges facing SDLs are multifaceted. Each contributor carries their biases and perspectives and may identify differing critical steps—such as deficiencies in AI, synthesis or characterization bottlenecks, a lack of APIs or standards, etc. If these shortcomings (shadows) can be taken holistically, the true core issues with SDL technologies (imaginary shape in the center) can be determined. Discerning the truth will require multiple perspectives and invites the potential for bringing AI analysts into the conversation. The community can then focus efforts and address what is truly critical.*

Concerning commercial equipment, preferential purchasing of equipment and software which provides native programmatic control is a good start. In purchasing agreements and vendor selection, the quality of their APIs, documentation, technical support, and data FAIR-ness can be emphasized to show that these resources are marketable. Furthermore, researchers should seek to engage with research and development departments to co-develop prototype automation tools. Even if these collaborative efforts cannot be promptly released, by having a seat at the table, gradual improvement to SDL integration can be achieved.

The SDL community must consider the technologies which it, itself, produces. How systems are made accessible to the broader research community can take multiple forms from low-cost/cost-shared solutions to open-access resources, to transparency and low technical knowledge interfaces. Groups currently developing SDLs should make an effort to reuse (or consult) as much code and data from prior studies as possible, even if it must be modified. While it is often beyond the scope of a single laboratory to develop robust, transferable code or experimental techniques, taking the time to analyze code and data reporting decisions can act as an additional form of dialogue between SDL developers. This encourages community involvement, reduces redundant effort, brings people into dialogue, and can help work out the bugs in our standardization efforts.

In improving the reporting of SDLs, the community will need better metrics than those currently used. While there is pressure to present research in the most flattering light while still being fair and honest, supplemental information needs to better characterize the reality of platforms in operations[39] (*e.g.*, its performance in well-defined tasks, devices, capabilities, and interfaces). The definition of (partial) success must be considered and discussed when reporting any metrics about SDL performance with respect to its objectives—*e.g.*, for a discovery campaign is there success in gaining any insights or only when a new compound is created and how do the properties of interest affect the degree of success? SDL reports should include calibrations, standards, and comparative or benchmarking studies performed so that others can better build off of the reported results. In addition, metrics such as overall operational performance, the degree of human involvement with the workflow, resources used and wastes generated, as well as an open discussion of areas where the platform could be reasonably improved should be reported (*cf.* ref. 175, ref. 176, and supplemental materials of ref. 3). Finally, economic or industry-aware analyses and discussions should be included whenever possible. Furthermore, each domain of science contributing to an SDL may come with its own idea of performance metrics—metrics that may require adjustment or reinterpretation in an SDL context. In robotics, metrics concerning the success of operations are muddied by a disconnect between high-level and low-level objectives; for example, when does the failure of a chemistry count as a failure of the automation? Reports of SDL advancements must make it clear exactly how success is defined, measured, and interpreted by both the researchers and the SDL's governing models. Ultimately, we want to help others learn from and interface with established SDLs, reduce redundant efforts between laboratories, and help collaborating research groups diagnose and troubleshoot irreproducibility problems.

While this list of reporting demands represents additional work in the present, it is important to establish rich descriptions of SDLs as the precedent for future work. This rigor will help to build and reinforce trust within and, perhaps more crucially, beyond the SDL community. Similarly, by having code and data available (when legal to do so), the communal development of SDLs can be accelerated and consensus can be achieved for best practices and a shared understanding of SDL language developed to propel SDLs into a democratized future. Additionally, rigorous reporting on SDLs, especially their shortcomings, establishes norms that not every published SDL needs to be flawless (an admission that helps the groups behind less "spectacular" SDLs to enter the conversation) and facilitates the identification of opportunities for improvement (inviting collaboration for perpetual improvement).

The user experience must also be considered. While potentially difficult to justify the expense of developing user interfaces (especially for research groups), a good user experience greatly improves the adoptability of the technology (especially for industry), lowers the barrier of entry for non-experts, and eases the friction caused by high generational turnover in academic groups. User interface design may require external support: an opportunity to collaborate with software developers outside of the SDL sphere, opening opportunities for undergraduate research and masters' theses and familiarizing more researchers with SDL technologies.

Proposals should be tailored to drive the diversification of collaborators. Diverse expertise supplies SDLs with the necessary breadth of knowledge required to be built and helps to foster and maintain collaborative relationships within the scientific and industrial communities so that future SDLs can thrive in a democratic and collaborative ecosystem. These cross-disciplinary collaborations will also facilitate the training of individuals in scientific communication and team science. Even when projects are simple, the inclusion of non-experts in SDL-related discussions helps prevent the gradual increase of the SDL skill-floor which often occurs when only experts are allowed to participate in discussions—outside (even naive) opinions help to challenge assumptions and bring in new ideas.

An institute for automated laboratory infrastructure could better focus the SDL community's efforts and provide partners with a meta-project with which to engage and interface. The NSF-funded, multi-university consortium, the Molecular Software Sciences Institute[177], which serves to enhance software-development efforts in the field of computational molecular science can act as a model. A consortium for SDLs would more readily sustain long-term funding to develop and maintain SDL software infrastructure (as opposed to specific hypothesis-driven research projects) as well as provide pre-competitive, non-proprietary support for academic and industrial researchers. Such a consortium could, as an external entity, attract long-term staffing who could cultivate a set of best-practices and engage in developing educational materials (online tutorials, in-person workshops) to train users. By focusing on core SDL issues, the tools developed in part of the consortium would serve both centralized and distributed SDL paradigms.

Acknowledgements
MA graciously acknowledges the financial support of the Technology, Innovation, and Partnerships (TIP) Directorate of the National Science Foundation (award #2332452) and the records made by Pragyan Jha, Fernando Delgado-Licona, Sina Sadeghi, and Nikolai Mukhin during the FUTURE Labs Workshop (NSF #2332452) at North Carolina State University. SVK was supported by the Center for Advanced Materials and Manufacturing (CAMM) and the NSF Materials Research Science and Engineering Centers (MRSEC). RGM acknowledges support from the INTERSECT Initiative as part of the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the US Department of Energy under contract DE-AC05-00OR22725. JS acknowledges support from the National Science Foundation (PHY-2226511, OAC-2320718).

Conflicts of Interest
JS is on the scientific advisory board of Atinary, mentioned in the article.

Refences
1. Chu, S. & Majumdar, A. Opportunities and challenges for a sustainable energy future. *Nature* **488**, 294–303 (2012).
2. Campos, K. R. *et al.* The importance of synthetic chemistry in the pharmaceutical industry. *Science* **363**, eaat0805 (2019).
3. Koscher, B. A. *et al.* Autonomous, multiproperty-driven molecular discovery: From predictions to measurements and back. *Science* **382**, eadi1407 (2023).
4. Tom, G. *et al.* Self-Driving Laboratories for Chemistry and Materials Science. *Chem. Rev.* **124**, 9633–9732 (2024).
5. Cosima Boswell-Koller *et al. Accelerated Materials Experimentation Enabled by the Autonomous Materials Innovation Infrastructure (AMII) A Workshop Report*. https://www.mgi.gov/autonomous-experimentation-materials-rd (2024).

6. B. Canty, R., A. Koscher, B., A. McDonald, M. & F. Jensen, K. Integrating autonomy into automated research platforms. *Digit. Discov.* **2**, 1259–1268 (2023).
7. Montoya, J. H. *et al.* Toward autonomous materials research: Recent progress and future challenges. *Appl. Phys. Rev.* **9**, 011405 (2022).
8. Sadeghi, S. *et al.* Engineering a Sustainable Future: Harnessing Automation, Robotics, and Artificial Intelligence with Self-Driving Laboratories. *ACS Sustain. Chem. Eng.* (2024) doi:10.1021/acssuschemeng.4c02177.
9. Grand Challenges - 14 Grand Challenges for Engineering. https://www.engineeringchallenges.org/challenges.aspx.
10. Stach, E. *et al.* Autonomous experimentation systems for materials development: A community perspective. *Matter* **4**, 2702–2726 (2021).
11. Baird, S. G. & Sparks, T. D. What is a minimal working example for a self-driving laboratory? *Matter* **5**, 4170–4178 (2022).
12. NSF BioPACIFIC MIP (DMR-1933487). https://biopacificmip.org/.
13. Masters, K. L. & Galaxy Zoo Team. Twelve years of Galaxy Zoo. *Proc. Int. Astron. Union* **14**, 205–212 (2019).
14. Khatib, F. *et al.* Crystal structure of a monomeric retroviral protease solved by protein folding game players. *Nat. Struct. Mol. Biol.* **18**, 1175–1177 (2011).
15. Hachmann, J. *et al.* The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid. *J. Phys. Chem. Lett.* **2**, 2241–2251 (2011).
16. NSF's 10 Big Ideas - Special Report | NSF - National Science Foundation. https://www.nsf.gov/news/special_reports/big_ideas/.
17. Seifrid, M. *et al.* Chemspyd: an open-source python interface for Chemspeed robotic chemistry and materials platforms. *Digit. Discov.* **3**, 1319–1326 (2024).
18. Wierenga, R. P., Golas, S. M., Ho, W., Coley, C. W. & Esvelt, K. M. PyLabRobot: An open-source, hardware-agnostic interface for liquid-handling robots and accessories. *Device* **1**, 100111 (2023).
19. Heckscher Sjølin, B. *et al.* PerQueue: managing complex and dynamic workflows. *Digit. Discov.* **3**, 1832–1841 (2024).
20. Politi, M. *et al.* A high-throughput workflow for the synthesis of CdSe nanocrystals using a sonochemical materials acceleration platform. *Digit. Discov.* **2**, 1042–1057 (2023).
21. Ziatdinov, M. A. *et al.* Hypothesis Learning in Automated Experiment: Application to Combinatorial Materials Libraries. *Adv. Mater.* **34**, 2201345 (2022).
22. Raghavan, A. *et al.* Evolution of ferroelectric properties in SmxBi1-xFeO3 via automated Piezoresponse Force Microscopy across combinatorial spread libraries. Preprint at https://doi.org/10.48550/arXiv.2405.08773 (2024).
23. Liu, Y. *et al.* Autonomous scanning probe microscopy with hypothesis learning: Exploring the physics of domain switching in ferroelectric materials. *Patterns* **4**, 100704 (2023).
24. Liu, Y. *et al.* Experimental discovery of structure–property relationships in ferroelectric materials via active learning. *Nat. Mach. Intell.* **4**, 341–350 (2022).
25. Roccapriore, K. M., Kalinin, S. V. & Ziatdinov, M. Physics Discovery in Nanoplasmonic Systems via Autonomous Experiments in Scanning Transmission Electron Microscopy. *Adv. Sci.* **9**, 2203422 (2022).

26. Pratiush, U., Funakubo, H., Vasudevan, R., Kalinin, S. V. & Liu, Y. Scientific Exploration with Expert Knowledge (SEEK) in Autonomous Scanning Probe Microscopy with Active Learning. Preprint at https://doi.org/10.48550/arXiv.2408.02071 (2024).
27. Bai, J. *et al.* A dynamic knowledge graph approach to distributed self-driving laboratories. *Nat. Commun.* **15**, 462 (2024).
28. Liu, Y. *et al.* Exploring the Relationship of Microstructure and Conductivity in Metal Halide Perovskites via Active Learning-Driven Automated Scanning Probe Microscopy. *J. Phys. Chem. Lett.* **14**, 3352–3359 (2023).
29. A. Leins, D., B. Haase, S., Eslami, M., Schrier, J. & T. Freeman, J. Collaborative methods to enhance reproducibility and accelerate discovery. *Digit. Discov.* **2**, 12–27 (2023).
30. Vogler, M. *et al.* Autonomous battery optimisation by deploying distributed experiments and simulations. Preprint at https://doi.org/10.26434/chemrxiv-2024-vfq1n (2024).
31. Gongora, A. E. *et al.* A Bayesian experimental autonomous researcher for mechanical design. *Sci. Adv.* **6**, eaaz1708 (2020).
32. Quinn, H. *et al.* PANDA: a self-driving lab for studying electrodeposited polymer films. *Mater. Horiz.* (2024) doi:10.1039/D4MH00797B.
33. Liu, Y. *et al.* Machine Learning-Based Reward-Driven Tuning of Scanning Probe Microscopy: Towards Fully Automated Microscopy. *arXiv.org* https://arxiv.org/abs/2408.04055v1 (2024).
34. Mehr, S. H. M., Craven, M., Leonov, A. I., Keenan, G. & Cronin, L. A universal system for digitization and automatic execution of the chemical synthesis literature. *Science* **370**, 101–108 (2020).
35. Darvish, K. *et al.* ORGANA: A Robotic Assistant for Automated Chemistry Experimentation and Characterization. Preprint at https://doi.org/10.48550/arXiv.2401.06949 (2024).
36. Ren, Z., Zhang, Z., Tian, Y. & Li, J. CRESt – Copilot for Real-world Experimental Scientist. Preprint at https://doi.org/10.26434/chemrxiv-2023-tnz1x-v4 (2023).
37. Gongora, A. E. *et al.* Using simulation to accelerate autonomous experimentation: A case study using mechanics. *iScience* **24**, 102262 (2021).
38. Snapp, K. L. *et al.* Superlative mechanical energy absorbing efficiency discovered through self-driving lab-human partnership. *Nat. Commun.* **15**, 4290 (2024).
39. Volk, A. A. & Abolhasani, M. Performance metrics to unleash the power of self-driving labs in chemistry and materials science. *Nat. Commun.* **15**, 1378 (2024).
40. Pence, M. A., Hazen, G. & Rodríguez-López, J. An automated electrochemistry platform for studying pH-dependent molecular electrocatalysis. *Digit. Discov.* **3**, 1812–1821 (2024).
41. Dixon, T. M. *et al.* Operator-free HPLC automated method development guided by Bayesian optimization. *Digit. Discov.* **3**, 1591–1601 (2024).
42. Liu, Y., Ziatdinov, M. A., Vasudevan, R. K. & Kalinin, S. V. Explainability and human intervention in autonomous scanning probe microscopy. *Patterns* **4**, 100858 (2023).
43. Pratiush, U. *et al.* Building Workflows for Interactive Human in the Loop Automated Experiment (hAE) in STEM-EELS. Preprint at https://doi.org/10.48550/arXiv.2404.07381 (2024).
44. Smith, S. C., Horbaczewskyj, C. S., Tanner, T. F. N., Walder, J. J. & Fairlamb, I. J. S. Automated approaches, reaction parameterisation, and data science in organometallic chemistry and catalysis: towards improving synthetic chemistry and accelerating mechanistic understanding. *Digit. Discov.* **3**, 1467–1495 (2024).

45. Emerald Cloud Lab: Remote Controlled Life Sciences Lab. https://www.emeraldcloudlab.com/.
46. German-Canadian Materials Acceleration Centre. https://gcmac.ca/.
47. CMU Cloud Lab | A Future of Science Initiative. https://cloudlab.cmu.edu/.
48. Arias, D. S. & Taylor, R. E. Scientific Discovery at the Press of a Button: Navigating Emerging Cloud Laboratory Technology. *Adv. Mater. Technol.* **9**, 2400084 (2024).
49. Office of Science User Facilities. *Energy.gov* https://www.energy.gov/science/office-science-user-facilities.
50. Automating Labs through Green Button Go | Biosero. https://biosero.com/ (2021).
51. Burke, M. D. *et al.* Molecule Maker Lab Institute: Accelerating, advancing, and democratizing molecular innovation. *AI Mag.* **45**, 117–123 (2024).
52. Li, J. *et al.* Autonomous discovery of optically active chiral inorganic perovskite nanocrystals through an intelligent cloud lab. *Nat. Commun.* **11**, 2046 (2020).
53. Kalinin, S. V. *et al.* Probe microscopy is all you need*. *Mach. Learn. Sci. Technol.* **4**, 023001 (2023).
54. Lo, S. *et al.* Review of low-cost self-driving laboratories in chemistry and materials science: the “frugal twin” concept. *Digit. Discov.* **3**, 842–868 (2024).
55. Beaucage, P. A. & Martin, T. B. The Autonomous Formulation Laboratory: An Open Liquid Handling Platform for Formulation Discovery Using X-ray and Neutron Scattering. *Chem. Mater.* **35**, 846–852 (2023).
56. Bach, U. & Leisten, I. How to Structure and Foster Innovative Research. in *Automation, Communication and Cybernetics in Science and Engineering 2009/2010* (eds. Jeschke, S., Isenhardt, I. & Henning, K.) 3–13 (Springer, Berlin, Heidelberg, 2011). doi:10.1007/978-3-642-16208-4_1.
57. Stokols, D., Misra, S., Moser, R. P., Hall, K. L. & Taylor, B. K. The Ecology of Team Science: Understanding Contextual Influences on Transdisciplinary Collaboration. *Am. J. Prev. Med.* **35**, S96–S115 (2008).
58. Bennett, L. M. Team Science: An Exercise in Difference and Diversity. in *An Astronomical Inclusion Revolution: Advancing Diversity, Equity, and Inclusion in Professional Astronomy and Astrophysics* (IOP Astronomy, 2024). doi:10.1088/2514-3433/ad2174ch8.
59. National Science Data Fabric. https://nationalsciencedatafabric.org/.
60. Pelkie, B. G. & Pozzo, L. D. The laboratory of Babel: highlighting community needs for integrated materials data management. *Digit. Discov.* **2**, 544–556 (2023).
61. AI research robots key to ‘democratizing and revolutionizing science’, world-class AFRL re. *One AFRL – One Fight* https://www.afrl.af.mil/News/Article-Display/Article/3559877/ai-research-robots-key-to-democratizing-and-revolutionizing-science-world-class/http%3A%2F%2Fwww.afrl.af.mil%2FNews%2FArticle-Display%2FArticle%2F3559877%2Fai-research-robots-key-to-democratizing-and-revolutionizing-science-world-class%2F (2023).
62. ARES Learning | Project-Based Research-Driven Space-Focused School & Enrichment. *ARES Learning* https://www.areslearning.com.
63. Saar, L. *et al.* The LEGOLAS Kit: A low-cost robot science kit for education with symbolic regression for hypothesis discovery and validation. *MRS Bull.* **47**, 881–885 (2022).
64. Epps, R. W. & Abolhasani, M. Modern nanoscience: Convergence of AI, robotics, and colloidal synthesis. *Appl. Phys. Rev.* **8**, 041316 (2021).

65. Gao, W. & Coley, C. W. The Synthesizability of Molecules Proposed by Generative Models. *J. Chem. Inf. Model.* **60**, 5714–5723 (2020).
66. Fromer, J. C. & Coley, C. W. An algorithmic framework for synthetic cost-aware decision making in molecular design. *Nat. Comput. Sci.* **4**, 440–450 (2024).
67. Wang, J. *et al.* ChemistGA: A Chemical Synthesizable Accessible Molecular Generation Algorithm for Real-World Drug Discovery. *J. Med. Chem.* **65**, 12482–12496 (2022).
68. Swanson, K. *et al.* Generative AI for designing and validating easily synthesizable and structurally novel antibiotics. *Nat. Mach. Intell.* **6**, 338–353 (2024).
69. Kalinin, S. V. *et al.* Designing workflows for materials characterization. *Appl. Phys. Rev.* **11**, 011314 (2024).
70. Strieth-Kalthoff, F. *et al.* Delocalized, asynchronous, closed-loop discovery of organic laser emitters. *Science* **384**, eadk9227 (2024).
71. Kusne, A. G. *et al.* On-the-fly closed-loop materials discovery via Bayesian active learning. *Nat. Commun.* **11**, 5966 (2020).
72. Maffettone, P. M. *et al.* Artificial Intelligence Driven Experiments at User Facilities. in *Methods and Applications of Autonomous Experimentation* (Chapman and Hall/CRC, 2023).
73. Aldeghi, M. *et al.* Roughness of Molecular Property Landscapes and Its Impact on Modellability. *J. Chem. Inf. Model.* **62**, 4660–4671 (2022).
74. Wang, T., Bao, C. & Shi, Z. Interface Laplace Learning: Learnable Interface Term Helps Semi-Supervised Learning. Preprint at https://doi.org/10.48550/arXiv.2408.05419 (2024).
75. Liu, H.-T. D., Williams, F., Jacobson, A., Fidler, S. & Litany, O. Learning Smooth Neural Functions via Lipschitz Regularization. in *ACM SIGGRAPH 2022 Conference Proceedings* 1–13 (Association for Computing Machinery, New York, NY, USA, 2022). doi:10.1145/3528233.3530713.
76. Luo, H., Demmel, J. W., Cho, Y., Li, X. S. & Liu, Y. Non-smooth Bayesian Optimization in Tuning Problems. Preprint at https://doi.org/10.48550/arXiv.2109.07563 (2021).
77. Skalse, J., Howe, N., Krasheninnikov, D. & Krueger, D. Defining and Characterizing Reward Gaming. *Adv. Neural Inf. Process. Syst.* **35**, 9460–9471 (2022).
78. Fromer, J. C. & Coley, C. W. Computer-aided multi-objective optimization in small molecule discovery. *Patterns* **4**, 100678 (2023).
79. Slautin, B. N. *et al.* Co-orchestration of multiple instruments to uncover structure–property relationships in combinatorial libraries. *Digit. Discov.* **3**, 1602–1611 (2024).
80. Batatia, I. *et al.* A foundation model for atomistic materials chemistry. Preprint at https://doi.org/10.48550/arXiv.2401.00096 (2024).
81. Slautin, B. N. *et al.* Bayesian Co-navigation: Dynamic Designing of the Materials Digital Twins via Active Learning. *ACS Nano* **18**, 24898–24908 (2024).
82. Seifrid, M. *et al.* Autonomous Chemical Experiments: Challenges and Perspectives on Establishing a Self-Driving Lab. *Acc. Chem. Res.* **55**, 2454–2466 (2022).
83. Fare, C., Fenner, P., Benatan, M., Varsi, A. & Pyzer-Knapp, E. O. A multi-fidelity machine learning approach to high throughput materials screening. *Npj Comput. Mater.* **8**, 1–9 (2022).
84. Zhan, N. & Kitchin, J. R. Model-Specific to Model-General Uncertainty for Physical Properties. *Ind. Eng. Chem. Res.* **61**, 8368–8377 (2022).
85. Kahle, L. & Zipoli, F. Quality of uncertainty estimates from neural network potential ensembles. *Phys. Rev. E* **105**, 015311 (2022).

86. Kapusuzoglu, B. & Mahadevan, S. Information fusion and machine learning for sensitivity analysis using physics knowledge and experimental data. *Reliab. Eng. Syst. Saf.* **214**, 107712 (2021).
87. Kirman, J. *et al.* Machine-Learning-Accelerated Perovskite Crystallization. *Matter* **2**, 938–947 (2020).
88. Moliner, M. *et al.* Application of artificial neural networks to high-throughput synthesis of zeolites. *Microporous Mesoporous Mater.* **78**, 73–81 (2005).
89. Stein, H. S. & Gregoire, J. M. Progress and prospects for accelerating materials science with automated and autonomous workflows. *Chem. Sci.* **10**, 9640–9649 (2019).
90. Desai, B. *et al.* Rapid Discovery of a Novel Series of Abl Kinase Inhibitors by Application of an Integrated Microfluidic Synthesis and Screening Platform. *J. Med. Chem.* **56**, 3033–3047 (2013).
91. Adamo, A. *et al.* On-demand continuous-flow production of pharmaceuticals in a compact, reconfigurable system. *Science* **352**, 61–67 (2016).
92. Ludwig, A. Discovery of new materials using combinatorial synthesis and high-throughput characterization of thin-film materials libraries combined with computational methods. *Npj Comput. Mater.* **5**, 1–7 (2019).
93. Yang, J. *et al.* Accelerating Materials Discovery by High-Throughput GIWAXS Characterization of Quasi-2D Formamidinium Metal Halide Perovskites. *Adv. Funct. Mater.* **n/a**, 2409293.
94. Higgins, K., Valleti, S. M., Ziatdinov, M., Kalinin, S. V. & Ahmadi, M. Chemical Robotics Enabled Exploration of Stability in Multicomponent Lead Halide Perovskites via Machine Learning. *ACS Energy Lett.* **5**, 3426–3436 (2020).
95. Soh, B. W. *et al.* Automated pipetting robot for proxy high-throughput viscometry of Newtonian fluids. *Digit. Discov.* **2**, 481–488 (2023).
96. Martin, K. N., Rubsamen, M. S., Kaplan, N. P. & Hendricks, M. P. Method for Interfacing a Plate Reader Spectrometer Directly with an OT-2 Liquid Handling Robot. Preprint at https://doi.org/10.26434/chemrxiv-2022-6z4q1 (2022).
97. Nazeri, M. *et al.* Leveraging Flexible Pipette-based Tool Changes to Transform Liquid Handling Systems into Dual-Function Sample Preparation and Imaging Platforms. Preprint at https://doi.org/10.26434/chemrxiv-2024-f67jg (2024).
98. Steiner, S. *et al.* Organic synthesis in a modular robotic system driven by a chemical programming language. *Science* **363**, eaav2211 (2019).
99. Vasquez, J., Twigg-Smith, H., Tran O'Leary, J. & Peek, N. Jubilee: An Extensible Machine for Multi-tool Fabrication. in *Proceedings of the 2020 CHI Conference on Human Factors in Computing Systems* 1–13 (Association for Computing Machinery, New York, NY, USA, 2020). doi:10.1145/3313831.3376425.
100. Siemenn, A. E. *et al.* Archerfish: A Retrofitted 3D Printer for High-throughput Combinatorial Experimentation via Continuous Printing. Preprint at https://doi.org/10.26434/chemrxiv-2024-fz16p (2024).
101. Ganitano, G. S., Wallace, S. G., Maruyama, B. & Peterson, G. L. A hybrid metaheuristic and computer vision approach to closed-loop calibration of fused deposition modeling 3D printers. *Prog. Addit. Manuf.* **9**, 767–777 (2024).
102. Hung, L. *et al.* Autonomous laboratories for accelerated materials discovery: a community survey and practical insights. *Digit. Discov.* **3**, 1273–1279 (2024).

103. Canty, R. B. & Abolhasani, M. Reproducibility in automated chemistry laboratories using computer science abstractions. *Nat Synth* (Accepted) doi:10.1038/s44160-024-00649-8.
104. Allan, D., Caswell, T., Campbell, S. & Rakitin, M. Bluesky's Ahead: A Multi-Facility Collaboration for an a la Carte Software Project for Data Acquisition and Management. *Synchrotron Radiat. News* **32**, 19–22 (2019).
105. Vescovi, R. *et al.* Towards a modular architecture for science factories. *Digit. Discov.* **2**, 1980–1998 (2023).
106. Digital Discovery Journal. *Royal Society of Chemistry* https://www.rsc.org/journals-books-databases/about-journals/digital-discovery/.
107. Monteith, J. Y., McGregor, J. D. & Ingram, J. E. Scientific Research Software Ecosystems. in *Proceedings of the 2014 European Conference on Software Architecture Workshops* 1–6 (Association for Computing Machinery, New York, NY, USA, 2014). doi:10.1145/2642803.2642812.
108. Freund, A. oss-security - backdoor in upstream xz/liblzma leading to ssh server compromise. https://www.openwall.com/lists/oss-security/2024/03/29/4.
109. Allec, S. I. *et al.* A Case Study of Multimodal, Multi-institutional Data Management for the Combinatorial Materials Science Community. *Integrating Mater. Manuf. Innov.* **13**, 406–419 (2024).
110. Scheffler, M. *et al.* FAIR data enabling new horizons for materials research. *Nature* **604**, 635–642 (2022).
111. Pendleton, I. M. *et al.* Experiment Specification, Capture and Laboratory Automation Technology (ESCALATE): a software pipeline for automated chemical experimentation and data management. *MRS Commun.* **9**, 846–859 (2019).
112. Bai, J. *et al.* From Platform to Knowledge Graph: Evolution of Laboratory Automation. *JACS Au* **2**, 292–309 (2022).
113. Pruyne, J., Wozniak, J. M. & Foster, I. Tracking Dubious Data: Protecting Scientific Workflows from Invalidated Experiments. in *2022 IEEE 18th International Conference on e-Science (e-Science)* 456–461 (2022). doi:10.1109/eScience55777.2022.00082.
114. Heid, E. *et al.* Chemprop: A Machine Learning Package for Chemical Property Prediction. *J. Chem. Inf. Model.* **64**, 9–17 (2024).
115. facebook/Ax. Meta (2024).
116. dragonfly/dragonfly. dragonfly (2024).
117. Noack, M. *et al.* gpCAM. https://doi.org/10.5281/zenodo.5975553 (2022).
118. scikit-learn/scikit-learn. scikit-learn (2024).
119. Hickman, R. *et al.* Olympus, enhanced: benchmarking mixed-parameter and multi-objective optimization in chemistry and materials science. Preprint at https://doi.org/10.26434/chemrxiv-2023-74w8d (2023).
120. Baird, S. G., Hall, J. R. & Sparks, T. D. Compactness matters: Improving Bayesian optimization efficiency of materials formulations through invariant search spaces. *Comput. Mater. Sci.* **224**, 112134 (2023).
121. AFRL-ARES/ARES_OS. AFRL-ARES (2024).
122. Atinary – Enables Self-Driving Labs® technology. https://atinary.com/.
123. Roch, L. M. *et al.* ChemOS: Orchestrating autonomous experimentation. *Sci. Robot.* **3**, eaat5559 (2018).
124. Sim, M. *et al.* ChemOS 2.0: An orchestration architecture for chemical self-driving laboratories. *Matter* (2024) doi:10.1016/j.matt.2024.04.022.

125. Tamura, R., Tsuda, K. & Matsuda, S. NIMS-OS: an automation software to implement a closed loop between artificial intelligence and robotic experiments in materials science. *Sci. Technol. Adv. Mater. Methods* **3**, 2232297 (2023).
126. Pruyne, J. *et al.* Steering a Fleet: Adaptation for Large-Scale, Workflow-Based Experiments. Preprint at https://doi.org/10.48550/arXiv.2403.06077 (2024).
127. M. Bran, A. *et al.* Augmenting large language models with chemistry tools. *Nat. Mach. Intell.* **6**, 525–535 (2024).
128. Boiko, D. A., MacKnight, R., Kline, B. & Gomes, G. Autonomous chemical research with large language models. *Nature* **624**, 570–578 (2023).
129. Ghafarollahi, A. & Buehler, M. J. ProtAgents: protein discovery via large language model multi-agent collaborations combining physics and machine learning. *Digit. Discov.* **3**, 1389–1409 (2024).
130. Tang, X. *et al.* Prioritizing Safeguarding Over Autonomy: Risks of LLM Agents for Science. Preprint at https://doi.org/10.48550/arXiv.2402.04247 (2024).
131. Kambhampati, S. *et al.* LLMs Can't Plan, But Can Help Planning in LLM-Modulo Frameworks. Preprint at https://doi.org/10.48550/arXiv.2402.01817 (2024).
132. Zhang, L., Merrifield, R., Deguet, A. & Yang, G.-Z. Powering the world's robots—10 years of ROS. *Sci. Robot.* **2**, eaar1868 (2017).
133. Juchli, D. SiLA 2: The Next Generation Lab Automation Standard. in *Smart Biolabs of the Future* (eds. Beutel, S. & Lenk, F.) 147–174 (Springer International Publishing, Cham, 2022). doi:10.1007/10_2022_204.
134. Rahmanian, F. *et al.* Enabling Modular Autonomous Feedback-Loops in Materials Science through Hierarchical Experimental Laboratory Automation and Orchestration. *Adv. Mater. Interfaces* **9**, 2101987 (2022).
135. jrlLAB/hardpotato. jrlLAB (2024).
136. Yoo, H. J. *et al.* Bespoke Metal Nanoparticle Synthesis at Room Temperature and Discovery of Chemical Knowledge on Nanoparticle Growth via Autonomous Experimentations. *Adv. Funct. Mater.* **34**, 2312561 (2024).
137. Roper, K. *et al.* Testing the reproducibility and robustness of the cancer biology literature by robot. *J. R. Soc. Interface* **19**, 20210821 (2022).
138. Hein, J. E. & Schrier, J. Guidelines for hardware-focused articles. *Digit. Discov.* **3**, 447–448 (2024).
139. Avoiding 'Bit Rot': Long-Term Preservation of Digital Information [Point of View] | IEEE Journals & Magazine | IEEE Xplore. https://ieeexplore.ieee.org/document/5768098.
140. Willoughby, C. & Frey, J. G. Data management matters. *Digit. Discov.* **1**, 183–194 (2022).
141. Maffettone, P. M. *et al.* What is missing in autonomous discovery: open challenges for the community. *Digit. Discov.* **2**, 1644–1659 (2023).
142. Clark, S. *et al.* Toward a Unified Description of Battery Data. *Adv. Energy Mater.* **12**, 2102702 (2022).
143. Szymanski, N. J. *et al.* An autonomous laboratory for the accelerated synthesis of novel materials. *Nature* **624**, 86–91 (2023).
144. Leeman, J. *et al.* Challenges in High-Throughput Inorganic Materials Prediction and Autonomous Synthesis. *PRX Energy* **3**, 011002 (2024).
145. Baird, S. G. & Sparks, T. D. Building a "Hello World" for self-driving labs: The Closed-loop Spectroscopy Lab Light-mixing demo. *STAR Protoc.* **4**, 102329 (2023).

146. Norquist, A. J., Jones-Thomson, G., He, K., Egg, T. & Schrier, J. A Modern Twist on an Old Measurement: Using Laboratory Automation and Data Science to Determine the Solubility Product of Lead Iodide. *J. Chem. Educ.* **100**, 3445–3453 (2023).
147. L. Snapp, K. & A. Brown, K. Driving school for self-driving labs. *Digit. Discov.* **2**, 1620–1629 (2023).
148. Services & Solutions • Frontage Laboratories. *Frontage Laboratories* https://www.frontagelab.com/services/.
149. Chemistry Testing Laboratory. *Certified Laboratories* https://certified-laboratories.com/chemistry/.
150. Vermeulen, B., Kesselhut, J., Pyka, A. & Saviotti, P. P. The Impact of Automation on Employment: Just the Usual Structural Change? *Sustainability* **10**, 1661 (2018).
151. Howard, J. Artificial intelligence: Implications for the future of work. *Am. J. Ind. Med.* **62**, 917–926 (2019).
152. The Science of Team Science | National Academies. https://www.nationalacademies.org/our-work/the-science-of-team-science.
153. GROWING CONVERGENCE RESEARCH (GCR) | NSF - National Science Foundation. https://new.nsf.gov/funding/opportunities/growing-convergence-research-gcr (2024).
154. Savage, N. Tapping into the drug discovery potential of AI. *Biopharma Deal.* (2021) doi:10.1038/d43747-021-00045-7.
155. Hede, K. PNNL Kicks Off Multi-Year Energy Storage, Scientific Discovery Collaboration with Microsoft. https://www.pnnl.gov/news-media/pnnl-kicks-multi-year-energy-storage-scientific-discovery-collaboration-microsoft (2024).
156. Umicore enters AI platform agreement with Microsoft. https://www.umicore.com/en/newsroom/umicore-enters-ai-platform-agreement-with-microsoft-to-accelerate-and-scale-its-battery-materials-technologies-development/ (2024).
157. Northvolt's embrace of machine learning. https://northvolt.com/articles/northvolt-machine-learning/ (2023).
158. Russo-Spena, T., Mele, C. & Marzullo, M. Practising Value Innovation through Artificial Intelligence: The IBM Watson Case. *J. Creat. Value* **5**, 11–24 (2019).
159. Cambridge and Google partner to facilitate AI research | University of Cambridge. https://www.cam.ac.uk/news/cambridge-and-google-partner-to-facilitate-ai-research (2023).
160. MIF Welcome Video. https://liverpool.cloud.panopto.eu/Panopto/Pages/Viewer.aspx?id=969aa046-7742-4f18-bfeb-b0730069a06c.
161. Bhowmik, A. *et al.* Implications of the BATTERY 2030+ AI-Assisted Toolkit on Future Low-TRL Battery Discoveries and Chemistries. *Adv. Energy Mater.* **12**, 2102698 (2022).
162. Acceleration Consortium. https://acceleration.utoronto.ca/.
163. CAPeX. https://capex.dtu.dk/.
164. Xu, L. D., Xu, E. L. & Li, L. Industry 4.0: state of the art and future trends. *Int. J. Prod. Res.* **56**, 2941–2962 (2018).
165. Home - Gaia-X: A Federated Secure Data Infrastructure. https://gaia-x.eu/.
166. Platform Industrie 4.0 (Homepage). https://www.plattform-i40.de/IP/Navigation/EN/Home/home.html.
167. Zhong, R. Y., Xu, X., Klotz, E. & Newman, S. T. Intelligent Manufacturing in the Context of Industry 4.0: A Review. *Engineering* **3**, 616–630 (2017).

168. Digital Innovation Facility - Institute of Digital Engineering and Autonomous Systems - University of Liverpool. https://www.liverpool.ac.uk/institute-of-digital-engineering-autonomous-systems/digital-innovation-facility/.
169. Adadi, A. & Berrada, M. Peeking Inside the Black-Box: A Survey on Explainable Artificial Intelligence (XAI). *IEEE Access* **6**, 52138–52160 (2018).
170. Miller, W. L. *et al. Integrated Research Infrastructure Architecture Blueprint Activity (Final Report 2023)*. https://www.osti.gov/biblio/1984466 (2023) doi:10.2172/1984466.
171. National Artificial Intelligence Research Resource Pilot | NSF - National Science Foundation. https://new.nsf.gov/focus-areas/artificial-intelligence/nairr.
172. INTERSECT | ORNL. https://www.ornl.gov/intersect.
173. Autonomous Discovery. *Argonne National Laboratory* https://www.anl.gov/autonomous-discovery.
174. Christensen, M. *et al.* Automation isn't automatic. *Chem. Sci.* **12**, 15473–15490 (2021).
175. Fakhruldeen, H., Pizzuto, G., Glowacki, J. & Cooper, A. I. ARChemist: Autonomous Robotic Chemistry System Architecture. in *2022 International Conference on Robotics and Automation (ICRA)* 6013–6019 (2022). doi:10.1109/ICRA46639.2022.9811996.
176. MacLeod, B. P. *et al.* Self-driving laboratory for accelerated discovery of thin-film materials. *Sci. Adv.* **6**, eaaz8867 (2020).
177. MolSSI – The Molecular Sciences Software Institute. https://molssi.org/.