Perspective

Engineering a Sustainable Future: Harnessing Automation, Robotics, and Artificial Intelligence with Self-Driving Laboratories

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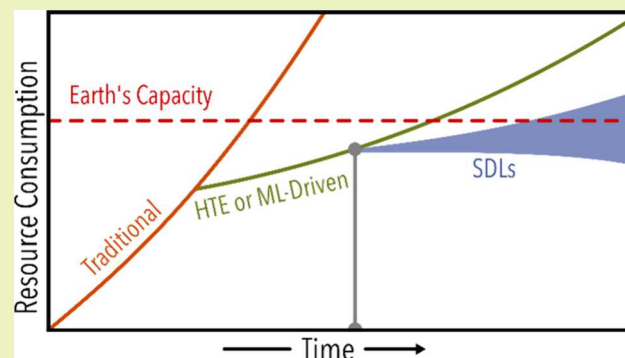
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ABSTRACT: The accelerating depletion of natural resources undoubtedly demands a radical reevaluation of research practices addressing the escalating climate crisis. From traditional approaches to modern-day advancements, the integration of automation and artificial intelligence (AI)-guided decision-making has emerged as a transformative route in shaping new research methodologies. Harnessing robotics and high-throughput automation alongside intelligent experimental design, self-driving laboratories (SDLs) offer an innovative solution to expedite chemical/materials research timelines while significantly reducing the carbon footprint of scientific endeavors, which could be utilized to not only generate green materials but also make the research process itself more sustainable. In this Perspective, we examine the potential of SDLs in

driving sustainability forward through case studies in materials discovery and process optimization, thereby paving the way for a greener and more efficient future. While SDLs hold an immense promise, we discuss the challenges that persist in their development and deployment, necessitating a holistic approach to sustainability in both design and implementation.

KEYWORDS: *sustainability, experimental design, automation, machine learning*

1. INTRODUCTION

The current global lifestyle consumes natural resources roughly twice as fast as the Earth can regenerate them.[1] Additionally, anthropogenic contributions to climate change have resulted in a global average temperature rise exceeding the Paris Agreement's 1.5 °C threshold for the first time in 2023.[2] As resource and health challenges become more complex, focusing solely on the "greenness" of a product is insufficient: the sustainability of the entire research, development, and production processes must be considered as well. Early efforts into sustainability focused on the economic optimization of production processes: using less material, generating less waste, and utilizing less hazardous materials.[3,4] Eventual efforts began to incorporate the product itself in the creation of materials which by their own action or by their contrast to existing materials are less harmful to (or actively beneficial for) the environment.[5,6] Irrespective of the final product, there is an opportunity to make materials discovery and process development research themselves more sustainable.[7] Considering Li-ion batteries and silicon-photovoltaics, technologies central to renewable energy efforts, these technologies have required decades of research from numerous laboratories to become
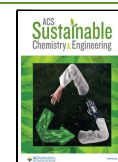
commercially viable and even longer to develop potential technological competitors. Automation and miniaturization already present a way to significantly reduce the carbon footprint of research and development,[8] and intelligent, collaborative research strategies enabled by artificial intelligence (AI) present the opportunity to reduce this carbon footprint further. Given the research acceleration possible with automation, AI, and collaboration, how would the Earth's biosphere and inhabitants benefit from industrially relevant, green alternatives to processes such as nitrogen fixation or materials such as concrete discovered and developed within the span of months rather than decades? As the demands for and complexity of higher-performing materials and increased process optimization grow, a new paradigm is needed for conducting sustainable research.

The concept of "sustainability" in a materials context is not new.[9,10] One of the earlier formal definitions from United Nations in 1987 was *"meet[ing] the needs of current generations without compromising the ability of future generations to meet their own needs"*,[11] yet with increased awareness of the hazards of petroleum and mining, it took on a sense of minimizing oil, plastic, and mined resources.[12] Then, the more modern idea of minimizing or offsetting carbon footprints arose around having a quantifiable means of measuring harm to the environment.[13,14] From this historical perspective, the complexity of achieving sustainability is shown as it requires minimizing harm (to an ever expanding network of, sometimes arbitrarily defined, human and natural systems), allocating resources, forecasting market demands, and predicting the cascade of both harm and technological capability. Regardless of the technical definition used, the reduction of material use, and the mitigation of hazards are central to engineering a sustainable future.

Within this broad context of sustainability, the field of chemical engineering, over the last two decades, has focused on improving chemical manufacturing processes and practices.[15,16] There is a nuance to the role of chemical engineering as a critical piece for the existing carbon-intensive chemical and materials industries. However, at its core, the desire to make the most of available resources (or renewable feedstocks) and promote safety have allowed chemical engineers to focus on improving dated chemical manufacturing techniques and make significant progress toward reducing the overall carbon footprint of chemical and material production processes.[16,17] Chemical engineering no longer addresses challenges of scale and throughput solely by making plants or laboratories larger; now environment-aware modeling, reactor engineering, and process optimization offer additional tools for scale-up. In addition to making production more material and energy efficient, the act of research has similarly seen material-conscientious optimization.[18] This intensification of research and production processes, both in academic and industrial settings, demonstrates the inherent ties of chemical engineering to sustainability—reflected in Anastas and Warner's 12 principles of green engineering,[19] the 5 principles of "Inherently safer design",[20] the adoption of numerous greener industrial processes,[21] and research practices utilizing automation.[22−24]

Tracing the evolution of scientific research from the Edisonian approaches to data-driven experimentation, the recent integration of machine-learning (ML) modeling and decision-making with process automation presents a powerful tool to more efficiently address current challenges facing the chemical industries[25]—such as those in materials development,[26] process optimization,[27] scale-up,[28] and translation to industry.[29] The potential of AI allied with automation and miniaturization is clear as a valuable tool to efficiently conduct sustainability research.[30−35] The synthesis of AI, robotics, and lab automation into a self-driving laboratory (SDL)[36] is a rapidly emerging concept by which research in chemical and materials sciences can be accelerated to meet these imminent challenges.[37−43] SDLs, by acting as a robotic copilot to the human researchers, can reduce the time to solution by a factor of 10−1000×,[44] compared to manual or semiautomatic experimental techniques—similarly, other explorations of manual, automated, and self-driving experimentation estimate 10−100× reductions in cost, waste, and energy.[8] The SDL's research acceleration is achieved by leveraging both high-throughput automation and intelligent experimental design/selection. This reduction of time, when combined with chemical engineering design frameworks such as process intensification, and green and circular chemistry principles, results in less material consumption and waste generation,[8] thus reducing the carbon footprint of the entire research workflow. To reduce redundant effort, it has been proposed to make the rich, digital experimental data sets generated by SDLs shareable such that the operation of one SDL catalyzes the education of other SDLs. It should be emphasized that while SDLs can (and should) be used to create green technologies/materials, this process of research is itself more sustainable than traditional high-throughput experimentation (HTE).

Within this Perspective, the anatomy of an SDL is dissected to evaluate the intrinsic sustainability of this autonomous research paradigm: the *process* rather than the *products* of SDLs' research. Next, examples of prototype SDLs' contributions to materials discovery and process optimization are provided to demonstrate the diversity of techniques and devices which can be integrated and the breadth of challenges these platforms can address. Finally, the remaining challenges of SDL development and deployment through the lens of sustainability are discussed.

2. SDLS: A ROBOTIC COPILOT FOR A SUSTAINABLE FUTURE

SDLs built through the integration of automated chemistry and material science laboratories with autonomy (automated decision-making) offer a promising avenue for different aspects of sustainability, ranging from the accelerated discovery of high-efficiency and clean energy materials to the optimization of material- and energy-efficient manufacturing processes (Figure 1). In addition to the material or process outputs of an SDL, the synergy of the physical and digital components of an SDL's experimentation can reduce the carbon footprint of
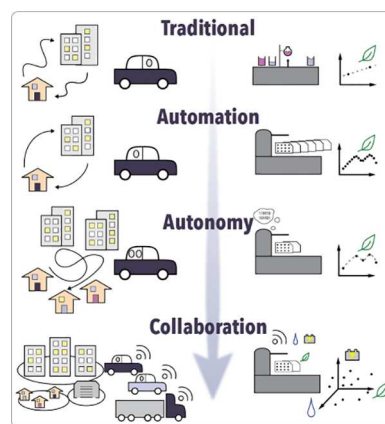

Figure 1. Analogy to self-driving vehicles to show the progression of experimental strategies. Traditional approaches are inefficient: the human driver selects routine paths, and the experimentalist obtains a paucal number of experiments. With automation, vehicles can find the most efficient paths and laboratories can conduct many experiments to exhaustively search a space. The introduction of autonomy further enhances efficiency: a fleet of self-driving cars can find optimal carpools and drastically reduce emissions; similarly a SDL can perform a minimal number of experiments while maximizing information gained. Finally, with the introduction of collaboration, multiple pathing or materials design needs can be addressed and distributed fairly to achieve optimality.
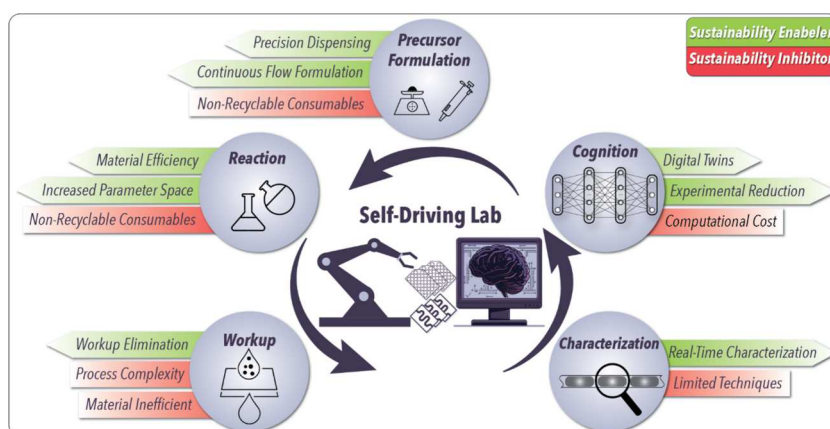
Figure 2. Breakdown of SDLs modules within the sustainability framework. Precursor preparation and the reaction module can benefit from miniaturization and on-demand material preparation. Synthesis and characterization should be designed synergistically to minimize the amount of workup necessary. Characterization should be data-rich to increase shareability and *in situ* to avoid throughput bottlenecks. The cognition module employs digital tools like ML-guided experimentation, models, and simulation to reduce the total number of physical experiments.

research itself. The physical and digital aspects must act in harmony to balance the costs of physical and computational experimentation. A resource-conscientious SDL may include miniaturized reactors, rapid online product analysis, and efficient optimization techniques. In this section, we discuss the physical and digital aspects of *green* SDLs—highlighting how these tools accelerate research and make research more sustainable.

Conventional human-dependent chemical and materials research and development in academic and industrial settings is rarely conscious of its impact on the environment. Traditionally, chemical synthesis relies on labor-intensive manual experimentation in batch reactors (e.g., flasks, autoclaves) which usually consume solvents and solids on the milliliter and gram scale per synthesis—leading to high chemical consumption and waste generation over an extended period of time. Additionally, one-factor-at-a-time or exhaustive combinatorial approaches to experimentation are slow at navigating through high-dimensional chemical spaces. Moreover, the segregation of the synthesis, characterization, and performance evaluation of materials results in the loss of intermediate information and opportunities for intersystem optimization (e.g., process control, heat recapture, reactive separations). The challenges of reproducing manual operations (with high variance and lossy data capture) hinders a smooth transfer of knowledge and necessitates further, redundant experiments—increasing chemical consumption, waste generation, labor costs, and project time. In the past three decades, lab automation technologies in chemistry and material sciences have been slowly evolving toward the goal of resource- and time-efficient development, resulting in HTE and reaction miniaturization. Building on the decades of advancements in laboratory automation technologies, SDLs seek to address the aforementioned challenges of the existing experimental sciences through optimal hardware and data engineering (Figure 2). The next subsections discuss various facets of SDLs and their role in making the overall experimental sciences more material- and time-efficient.

2.1. Precursor Formulation Module. Batch-to-batch precursor variability imposes a prevalent challenge to the chemical synthesis. Consistent precursor compositions are a prerequisite for reproducible synthesis. The precursor variability challenge lies in the variation during solid and liquid dispensing as well as in mixing. The automation of material handling provides improved accuracy and precision over manual preparation, and the standardization of solution processing diminishes concentration and temperature variations, resulting in improved precursor reproducibility.

Commercial liquid-handling robots have provided general and highly specialized automated options for microliter-level liquid dispensing in the life sciences[45] and are seeing increased use in chemical and materials science research.[46] Do-it-yourself and 3D-printed pipetting robots are drawing increased attention due to their low-cost and reconfigurability.[47] Discrete and continuous liquid handling are enabled via common and reliable liquid transfer tools such as syringe and peristaltic pumps, and automation interfaces allow these tools to be readily connected into SDLs.[48] The automation of small-scale solids handling, however, is stymied by challenges with managing and accounting for particle size distributions, static, and moisture—variables which result in inconsistent dispensing and mechanical bugs.[49] Commercial solid dispensing robots typically rely on gravity, hoppers, or positive displacement to dispense solids and on precise calibrations or gravimetric sensors to determine the amount of material dispensed.[50] Recently, a biomimetic dual-arm solid dispensing robot with a lower operating bound for 2 mg dispenses was published.[51]

The automation of heating, cooling, and mixing steps also helps to reduce precursor variability. Heating and cooling modules, either integrated with pipetting robots or working independently, offer precise and uniform temperature control across the reactor (or batch of reactors as in a well plate).[52,53] Mixing modules (typically shakers for well plates or stirrers for sealed reactors) can provide adequate mixing for many applications—achieving uniform and rigorous mixing in well plates remains an open challenge.[54] Crucially for the objective of reproducibility (the reduction of replicate experiments and their material use and waste generation), the reliability and capability of these formulation modules can be resolved with technological advancements that can be easily rolled out *en masse*—in comparison to the (re)training of human operators.

2.2. Reactor Module. The reactors play a vital role in the quality of synthesis, experimental throughput, and material consumption. The most common reactor is a single batch reactor, which can be a vial, a flask, or a beaker. Single batch

reactors are compatible with many general-purpose pipetting machines and robotic arms. However, even small single batch reactors consume milliliter quantities of material, and their size can result in concentration and temperature gradients which may hinder process optimization or intensification.

Miniaturized batch reactors, such as multiwell plates, increase throughout while reducing the chemical consumption per reaction and retain their compatibility with many well-established automation technologies such as liquid handlers and robotic arms. Miniaturized batch reactors can handle solids and suspensions during synthesis relatively easily[55] (cf. flow reactors) and are suitable for dealing with discrete reaction parameters in parallel (such as in catalyst and biomolecules screening campaigns[56,57]). SDLs utilizing batch reactors can leverage the free transfer of material between unit operations (e.g., a robotic arm ferrying samples between analytical devices) to enable flexible, parallelizable workflows and facilitate the incorporation of new unit operations with minimal integration effort. Resource efficiency in plate-based architectures is, however, curtailed by the material waste generated (sc. multiwell plates and pipetting tips). Multiwell plates are typically made of polystyrene and polypropylene, which are nonrecyclable especially when contaminated by reaction materials, and can result in high carbon footprints for platforms which operate continuously for long periods of time. This waste generation motivates the transition from exhaustive HTE to the intelligent experiment selection and reaction plating of SDLs to minimize the number of experiments, and thus multiwell plates and tips used.

Due to their facile integration to automated workflows, microfluidic reactors have been widely utilized in SDLs for continuous HTE.[58,59] Microfluidic reactors enable continuous control of reaction conditions (such as reaction temperature, residence time, and precursor flow rates) allowing for rapid switching between experimental conditions. This reduced downtime for cleaning and equilibration translates into less waste and less starting material which improves the material efficiency of operation.[60] Microfluidic reactors, in comparison to batch reactors, minimize heat- and mass-transfer artifacts, which in turn improves the quality of reaction data and facilitates the exploration of reaction spaces. Single-droplet and multiphase, segmented flow strategies further reduce material use and enhance mixing, boosting throughput and offering an economic edge for organic and nanoparticle synthesis.[60] While flow reactors synergize well with SDLs, they are challenged by solids, the coupling of experiments conducted in series, and often require substantial development time. Recent efforts have been successful in making microfluidic systems more modular to improve their flexibility;[61] however, in some applications other architectures are more appropriate.

Future SDLs may consider reactor design as a free parameter during research. Recent efforts have been made to have SDLs 3D print reactors as needed,[62,63] and it is possible to have an SDL overcome the challenges of batch or flow architectures by integrating both approaches and selecting the optimal configuration for experimentation. Moreover, with the integration of *in situ* sensors (for typical reactor process variables such as temperature and pressure; for characterization, see Characterization Module), reactor conditions could be modified in real time to provide better control and enriched data extraction and to accelerate exploration based on meta-experimental information (e.g., avoiding conditions which cause clogs or which are hard to control).

2.3. Workup Module. The crude reaction mixture exiting the reactor module requires workup before the results can be characterized as the reaction effluent may contain the target product, byproducts, and unreacted reagents. Typical benchtop approaches such as column chromatography, filtration, and extraction often require copious amounts of solvent to isolate products and subsequent reconcentrating steps and must be followed with *ex situ* analysis for the identification and quantification of each component.

Versions of many isolation, purification, and workup approaches have been demonstrated in automated experimental systems: filtration, membrane filtration, gravity-based separation, centrifuges, liquid–liquid extraction, high-performance liquid chromatography (HPLC), lyophilization, dilution/concentration, solvent changes, annealing, deposition, quenches, and pretreatments.[64–67] Further integrations with mass spectrometry, nuclear magnetic resonance spectrometry (NMR), and Fourier-transform infrared spectrometry have been used to assist in robust isolation—in addition these techniques are used to verify the identities of products and can permit the precise calculation of reaction yields and selectivities. Despite the diversity of separation techniques, their automation and full integration into SDLs has remained a challenge. Separation techniques typically require fine-tuning/calibration for optimal performance (which may not be possible in discovery applications) and their physical interfaces may require changing between batch and flow paradigms. Moreover, current automation approaches have required specialized programmatic interfaces or the automation of human-centric interfaces.

Industrial wisdom indicates that the ideal process workup is to not need it at all: by achieving sufficient yield and selectivity through processes intensification that the question of subsequent isolation and purification is moot. While SDLs cannot rely on this approach (they are the means by which those optimal, intensified reaction conditions are achieved), they stand as an opportunity to deeply integrate both synthesis and isolation processes together—using data from one to inform the other. This collaboration between the reactor and workup modules could further improve the efficiency of the research platform by reducing time and waste generation.

2.4. Characterization Module. Automated characterization is central to closed-loop SDLs as it controls the accuracy and richness of the experimental data provided to the governing ML agents. The in-line or *in situ* characterization of reaction products provides real time analysis of the tested experimental condition(s), enables the analysis of transitory periods between experiments and enriches the acquired data set. Depending on the application, multiple characterization techniques (encompassing different physicochemical, structural, and/or optical properties of the reaction product, for example) are required to provide sufficient information to the ML agents.

When exploring organic compounds, chromatography-based characterization techniques (e.g., gas chromatography, HPLC), coupled with a variety of detectors such as ultraviolet/visible (UV/vis) absorption and MS, are common commercially available separation and quantification techniques.[68–71] However, the duration and discrete-sampling of chromatography-based techniques may lag behind the throughputs of other modules. This disparity of throughputs can result in the underutilization of other modules in an SDL, reducing the platform's overall time-efficiency.

Spectroscopic analyses—such as NMR, Infrared, and UV/vis—can be performed *in situ* via flow cell or probes to indicate material identities or measure electronic transition properties.[39,72−74] Recent developments toward automated microscopy could lead to SDLs with real-time imaging analysis for the shape and size characterization of materials.[75,76] The automation of sensors for live feedback, while useful for robust HTE platforms, is crucial for the maturation of SDLs as it permits not only the generation of data-rich experimental observations but also provides meta-data about the techniques and methods of the SDL's operation—potentially enabling SDLs that can learn and develop better experimental techniques.

Nevertheless, the available chromatography and spectroscopy technologies have not kept pace in the past decade, impeding the propagation of SDLs. For example, high-throughput structural characterization for inorganic materials (such as X-ray diffraction) is still difficult, slowing advances in SDLs for inorganic materials. While the macroscopic side of materials science SDLs have seen mechanical construction and testing workflows becoming increasingly automated,[77,78] nanomaterial characterization is lagging.

Many of the existing characterization tools can fall into the trap of being used to accelerate the Edisonian approach: reducing the time to solution and reducing material used per reaction yet permitting disproportionately more experiments—diminishing their potential to enable sustainable research workflows. Given the potential throughputs of SDLs, characterization techniques will need to be made more sensitive (requiring less material for good signal) and less destructive (reducing the demands on synthesis and workup) to fully enable the power of SDLs in the context of efficient research. Automation-amenable characterization techniques are urgently needed for the proliferation of SDLs.

2.5. Cognition Module. SDLs integrate and leverage multiple digital technologies to improve efficiency, accuracy, and reproducibility toward the goals of the experimental design and its execution. It could be argued that the greenest approach for accelerated experimentation is not experimentation at all: ideally, prior knowledge and theory, combined with modeling, should synthesize the solution before a physical experiment is ever performed. In practice, iteration is necessary to overcome uncertainty and deficiencies in current models and theories. SDLs, then, represent an effort to find, given the costs and benefits of each, the optimal balance between *thinking* about problems and *doing* experiments.

An SDL can leverage simulation and modeling to supplement experiments, ML agents to conduct experiments, and data-mining to augment training sets. The use of models and simulation, such as the use of density functional theory (DFT) to conduct virtual experiments, reduces the total number of physical experiments required[79,80] and can aid in the generality of SDLs to new applications. For example, Strieth-Kalthoff et al. were able to integrate a four-step DFT process into their workflow for the discovery of organic laser emitters where in the last step the predicted ground- and excited-state energy gradients were used to optimize structures and eliminate entire sections of the parameter space.

The use of purely *in silico* experimentation would eliminate the use of potentially scarce, costly, or hazardous precursors, waste, and any unsafe operational conditions. However, the realization of experiments identified purely through digital screening may encounter subsequent feasibility constraints.

Thus, physical experimentation must be made general, so as to not artificially restrict proposed experiments and must be able to perform probing and validation experiments at pace with the digital experimentation. For successful *in silico* strategies,[81,82] large amounts of reliable and varied data are essential.

Beyond theory-based modeling, the ML agents of an SDL require substantial quantities of high-quality data in order to operate effectively. In recent years, data-mining approaches such as large language models[83] and graph neural networks (GNNs)[84] have shown to be quite effective at extracting knowledge from unstructured literature formats. This enables an SDL to not only generate initial data sets on which to train its ML agents but also affords the ability to reference the literature during operation as would a scientist and avoid redundant or wasted effort.

Prepared with ML agents, SDLs can design experimental campaigns that are more efficient than human-generated or combinatorial campaigns at generating information per experiment—reducing the expected number of experiments before success and increasing the probability of the autonomous experimental campaign's success.[77,85,86] An added advantage of ML-guided experimentation is that, with proper incentivization and training, experimental campaigns can be designed to include additional factors such as material use, waste generation, atom economy, and hazard mitigation.

The digital world of SDLs also extends to process automation and coordination, such as remote and collaborative experimentation between SDLs to reduce redundancy and material transfer between laboratories[87] and the management of data in sharable and usable formats for effective and efficient collaboration. The virtualization of experiments and collaboration is not free, however, as it relies on extant (and may incur the creation of new) networks, data storage systems, and data processing centers. These entities can involve considerable resources (particularly electricity and water[88]). To some extent, the digital carbon footprint of SDLs can be mitigated through the use of carbon-neutral power sources; however, both the design of SDL infrastructure[89] and the computational- and data-efficiency of the models/software using them must be addressed.

Process automation and orchestration streamlines operations—optimizing resource utilization and enabling parallelization.[90,91] Multiple open-access orchestration platforms have been designed to help with communication between hardware.[92−94] Sim et al. introduced ChemOS 2.0, which is an orchestration architecture that coordinates the communication, exchange of data, and instruction management among instruments. Orchestration beyond a single lab allows for remote and collaborative experimentation. This allows laboratories to distribute effort, leverage specialized equipment or rare resources without requiring transportation, and pool resources into efficient, integrated facilities.[80,95] This enhances accessibility to SDL technologies and reduces the burdens of constructing and maintaining an individual SDL.

Within the digital aspect of SDLs, the computational method plays a vital role in optimizing or discovering materials. Optimization techniques are pivotal in achieving sustainability objectives in chemistry and materials science. Single-objective optimization focuses on finding the best solution to a given problem from a set of possible solutions, typically defined by a single output or a scalarization of multiple outputs. Multiobjective optimization, on the other hand, focuses on finding the best trade-off between competing output parameters.

Furthermore, choosing the appropriate optimization technique can be challenging when dealing with multiple considerations such as the number of experiments, computational cost, sizes of the input and output spaces, and performance metrics. In recent years, algorithm benchmarking has gained popularity to help future researchers decide which algorithms work best for a particular project.[85,96]

3. EXAMPLES OF SDLS FOR SUSTAINABILITY

Synergy between physical and digital aspects of SDLs will drive acceleration to shorten the time to solution of various sustainable development goals, including affordable and clean energy, responsible consumption and production, good health and well-being, clean water and sanitation, climate action, among others.[97] Several proof-of-concepts SDLs have succeeded in the discovery of novel materials and molecules for specific domains—e.g., solid electrolytes, proteins, electrocatalysts, thin film materials, and quantum dots (QDs)[98−101]— and in green-minded process design and optimization—e.g., photocatalysis,[28] catalytic[102,103] and chemical reactions,[97] and materials manufacturing.[104] However, few calculate the relative material/energy use compared to non-self-driving research strategies or use sustainability metrics to guide experimentation (Table 1). With continued development addressing the

Table 1. Extant SDL or Autonomous Laboratory Systems or Tutorials[a]

Gesture	Quantification	Guide	Both
64 (60.3%)	32 (30.8%)	6 (5.8%)	4 (3.9%)

[a]In a survey of 106 manuscripts on extant SDL or autonomous laboratory systems or tutorials, while many gesture toward sustainability, produce "green" materials, or optimize processes, (gesture) only a handful explicitly calculate sustainability metrics (quantification) or use such metrics to guide experimentation (guide). Counts are presented with a relative percent below in parentheses (accounting for some manuscripts that were deemed not applicable for individual classifications).

physical and digital components of SDLs, the next generation of SDLs must be able to handle both materials and molecular discovery and the optimization of workflows such that the research itself, not just the product, is also sustainable.

In order to engineer a sustainable future, new high-performing eco-friendly materials along with green manufacturing technologies will be required. To this end, discovery efforts have attempted to accelerate the rate at which new functional materials, which can be used to address current and future challenges, are created. In addition to material discovery, SDLs represent a transformative approach for process optimization. These "processes" may include chemical reactions, separations (such as distillation), remedial treatments (such as carbon capture), recycling, or entire chemical/material manufacturing production lines. SDLs provide a continuous, iterative route to automate material discovery and process optimization by designing and testing new materials and approaches and leveraging data-driven insights extracted from each experiment to efficiently explore chemical and design spaces.

With the growing demand for renewable energy sources, greener synthesis pathways, and environmentally friendly manufacturing processes compounded with the growing complexity of material solutions, sustainability goals, resource conservation, and responsible and environmentally conscious practices across scientific research and industrial sectors, neither scaling-out nor intelligent design of experiments alone will suffice. In this section, we illustrate how the pace of scientific discovery and development is being accelerated by SDLs to meet these demands.

3.1. Discovery: Finding the Solutions of Tomorrow. SDLs take advantage of the synergy between physical and digital components referenced above to tackle problems with intractable parameter spaces, such as synthesis of inorganic materials. Symanski et al., developed an SDL for the solid-state synthesis of air-stable oxides and phosphates for electronics.[105] It orchestrated a robotic platform to perform selected chemistries found in the Materials Project database. Since the chemistry was unknown, synthesis recipes were proposed after analyzing literature by natural-language models. Active learning was applied to direct the feasibility of each target material and resulted in the purported discovery of 41 novel materials in 17 days—notably, however, criticism of the validity of these materials while this manuscript was under review[106] underscores the critical need for benchmarking and cross-validation in SDL workflows.

Present high-throughput virtual screening approaches suffer from a limited pool of materials and the high computational cost of modeling calculations.[107] Consequently, the use of ML models, such as GNNs,[84,108,109] have been employed to explore the vast chemical space. Another popular strategy for accelerated materials and molecular discovery is inverse design. Polykovskiy et al., applied a generative model, to propose a novel inhibitor of Janus kinase 3.[110] This is made possible by encoding the high-dimensional chemical space into a continuous latent space of lower dimensionality, facilitating the generation of new molecules with target properties using the knowledge contained in this latent space. The generated molecule was later synthesized and tested in vitro, significantly increasing the time and atom efficiency of the typical drug discovery cycle.[111]

Digital twins provide a model of the real system as the basis for experimental selection and design. *SmartDope*[85] is an SDL for the production of QDs that uses an ensemble of neural networks to model the relationship of synthesis parameters and QD properties to enable experimental selection through Bayesian optimization (BO). The SDL was able to discover the best-in-class doped metal halide perovskite QD of its search space (of $\sim 10^{13}$ possible synthesis conditions) within only 1 day of continuous, automatic experimentation. Leveraging continuous experimentation and *in situ* characterization, *SmartDope* accelerated materials discovery for renewable energy technologies.

By discovering novel materials, future generations are provided with a greater arsenal of materials, tools which can be used to address the problems they face. By making the discovery of these materials resource- and waste-efficient, those generations will start from a lesser deficit, and have more resources and knowledge available to optimize the production of these solutions.

3.2. Process Optimization: Making the Most of the Solutions of Today. Optimizations, especially those for scale-up, are instrumental in both industrial adoption and the

reduction of industrial carbon footprints. Through the use of advanced data analytics and real-time process monitoring, SDLs can identify inefficiencies in processes and implement corrective measures to improve overall performance.

In the past few years, SDLs have been successfully deployed for both accelerated discovery of greener materials and process optimization of environmentally friendly manufacturing routes. For instance, the open-source, autonomous platform, Robo-Chem,[28] integrates a liquid handler, syringe pumps, a photoreactor, affordable Internet of Things devices, and an in-line benchtop NMR spectrometer to facilitate automated and data-rich optimization of photocatalytic transformations such as photoredox catalysis. By utilizing a combination of robotic automation and algorithmic optimization, RoboChem streamlines the process of reaction optimization and scale-up, reducing the need for human intervention. This not only enhances operational safety but also enables researchers to dedicate more time to creative aspects of chemistry, ultimately fostering innovation in sustainable chemical processes. Additionally, the platform's modularity allows for integration with various reactors and analytical technologies, enhancing versatility in addressing diverse challenges.

Braconi et al. utilized BO to identify reaction conditions with earth-abundant catalysts and nonhazardous solvents, particularly for the case of C−N coupling of sterically hampered bromo-pyrazines and benzylamines.[112] The BO approach efficiently explored a 140k-reaction space with only 80 experiments while achieving 87% yield. This BO approach was then combined with design of experiment models to provide a richer analysis to the researchers. Similarly, through the use of a multiobjective BO algorithm, robotics, and automated data-rich experimentation, Nambiar and co-workers presented a robotic platform to optimize computer-generated synthesis plans for the small molecule pharmaceutical, sonidegib. In this study, the authors highlighted the importance of human input for addressing unforeseen chemical incompatibilities and refining synthesis strategies. These examples demonstrate how machine assistance streamlines process optimization, and how researchers can shift focus to underlying chemical and physical processes, ultimately facilitating the development of better (broadly applicable) approaches in the future.[61]

Bridging optimization and discovery, the modular robotic SDL, Ada, autonomously optimized the optical properties of thin film materials by adjusting the composition and processing conditions. By automating experimentation processes and enhancing adaptability through modularity, the Ada platform accelerated material development, potentially leading to new solutions for advanced solar cells and other applications. Furthermore, the platform's scalability and ability to accommodate diverse materials and techniques offered a pathway for broader adoption within the materials science community.[101]

4. CHALLENGES AND OPPORTUNITIES

The power and potential of SDLs may be clear, but SDLs are held back from driving into a sustainable future due to the technological restraints. Much of the fundamental experimental machinery used by SDLs was developed for biology and not chemistry/materials science and may not be compatible with the necessary engineering controls imposed by reactive materials. As many synthesis, workup, and characterization technologies were designed in isolation, there are challenges in

matching throughputs; in addition, commercial automation interfaces are often lacking in the level of control required for research and deep integration into an SDL and creating software wrappers to supplement these interfaces requires great technical expertise.[113] These problems are tangential to the core of why SDLs are not already the common research paradigm. SDLs promise a reduction in material use and time spent finding solutions, fundamentally by reducing redundant and unnecessary experimentation; furthermore, SDLs promise a self-perpetuating cycle of collaborative research to address problems of increased complexity and scale. These promises, however, are locked behind by a lack of communication of performance metrics for each developed SDL.

Redundant experiments are avoided by the transparent and rapid communication of experimental plans and results as well as by more precise equipment. The current fleet of SDLs has been, however, developed in isolation as a result of funding interests with specific foci and the current atmosphere in academia to be quick to publish. This need for speed results in prototype SDLs with hardware limitations that may corrupt experimental results (e.g., such as optima lying beyond operational conditions) and in highly specialized units that do not generalize to other applications. As a consequence, an SDL may not be able to utilize data generated on another SDL, resulting in redundant experiments. Even with otherwise reliable data generation, documentation, and reporting, intellectual property restrictions can prevent the communication of these results and (software) tools used to aid in autonomous operation.[114] SDLs also may strain existing (meta)data formats such as FAIR[115] due to the convolution of experimental, platform, and environmental information.[116,117] This difficulty in communicating results and tools causes friction that hinders the self-perpetuation of SDLs.

SDL technologies are only useful toward elevating the quality of human life and maintaining natural resources insofar as they are used. The deployment of SDLs can be challenged by the presence of "bigger problems" (such as electricity production, transportation emissions, and food and water scarcity). However, SDLs provide the fundamental research needed to address those very problems. By accelerating (and lessening the carbon footprint of) research, SDLs help find ways around and solutions to these big problems. SDLs need a champion demonstration of their capabilities in an industrially relevant problem to ignite interest that will propel them into use in the future.

Even with the expectation that the barrier to entry for SDLs will decline over time, because SDLs are expensive to build but provide more cost-effective research, they can cause disparity in research capability (and thus funding) between the laboratories with and laboratories without an SDL.[118,119] Such disparities can deter a willingness to collaborate (again increasing the probability of redundant efforts) and can pose a risk of skill erosion in the workforce (hampering scientists ability to address future problems). Moreover, the desire to break into the SDL scene despite the barriers can result in *ad hoc* solutions to solved problems, circling back to the issues of poor reproducibility and generalizability which prevent SDLs from delivering on their promise to reduce wasted effort.

Due to a lack of standardization in measuring and reporting SDL performance metrics, the scientific community lacks the ability to effectively communicate about and thus improve SDLs. Without proper metrics, it is hard to determine the transferability of SDLs across the material-scale and data

boundaries between research institutions and industry partners (cf. disparities in the size, format, detail, rights, etc., of data available to each). Moreover, as SDLs are complicated systems in an ecosystem without good metrics for describing them, it can be hard to forecast platform needs when designing them.[54] This can often result in wasteful solutions. On the hardware side, it is easy to oversize throughput needs which can make an SDL just as wasteful as a traditional HTE platform. On the software side, it is easy to deploy unnecessarily involved ML agents that waste computational resources[120] and may be oversized for the data set and rate of data generation available, ultimately resulting in poorly trained or overfit models.[121] The poor generalizability of these models results in worse performance and reduced transferability—breaking the promises of more efficient experimentation.

Furthermore, as complicated systems with limited vendor support for automation and personnel training in automated research and ML, many SDLs face challenges with maintenance.[54] Discovery-oriented platforms especially face challenges with new conditions and materials causing problems (clogs, fires, signal aberration, etc.) which can necessitate resource-intensive cleaning, discarded experiments, and time-consuming platform rectification. Ultimately, the inclusion of such maintenance metrics into reporting on SDLs will enable pain-points to be identified, engineering solutions to be developed, and the overall usability of SDLs to be improved—moreover, these metrics will be crucial for adoption by industry where having realistic estimates for downtime and maintenance costs are crucial for evaluating investment in projects.

At the core of these roadblocks preventing SDLs from fulfilling their promise of creating a more sustainable research paradigm is a lack of communication. There is a need for more useful metrics to better understand the economic and ecological impacts of SDL operation.[122] Furthermore, universal standards for hardware and software interfaces are required to reduce redundant efforts in the construction of SDLs and the integration of SDLs into a collaborative network. To provide for the development and measurement of the benchmarks and interfaces, it may be necessary to push for incorporating into grant proposals sections on sustainability to ensure there are measured deliverables.

Incorporating sustainability metrics such as life cycle assessment (LCA), and technoeconomic analysis (TEA), and measures of adherence to the 12 principles of green chemistry into materials discovery, process optimization, and self-monitoring workflows is essential for transparent communication of SDL technologies.[17] These frameworks provide a systematic approach to evaluating and minimizing the environmental impacts of products and processes. LCA allows for a comprehensive analysis of the environmental impacts associated with a product or process throughout its entire life cycle, from raw material extraction to end-of-life disposal.[123,124] By integrating metrics such as LCA into the process optimization and materials flow into the discovery framework of SDLs, scientists can assess the environmental footprint of experimental designs and identify opportunities for improvement. By quantifying resource consumption, energy use, emissions, and other environmental factors, LCA enables the automation of decision-making strategies and the evaluation of potential alternatives. TEA evaluates the holistic economic viability (such as input, output/waste, and operational costs as well as output returns) and facilitates the transfer of SDLs and

their outputs (materials or processes) to industry.[125] Metrics for the adherence to the 12 principles of green chemistry allow ML agents to approach the design of materials and processes with sustainability in mind. These principles and metrics guide researchers and engineers in designing chemical processes and products that minimize waste, reduce toxicity, conserve resources, and promote safer alternatives. By codifying the way by which SDLs adhere to these principles into measurable observables, these platforms can steer toward long-term environmental objectives and communicate their progress to collaborators, robotic, academic, industrial, or otherwise.[126] With this breakthrough for communication, and thus collaboration, SDLs can contribute fully to the development of more sustainable technologies and practices, driving positive change to both the way research is conducted and to the solutions research provides.

■ ASSOCIATED CONTENT

ⓢ Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.4c02177.

Keywords, purview, exceptions, screening, measures, and survey of self-driving lab literature (Table S1), (PDF)

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Notes

The authors declare no competing financial interest.

Biographies

Sina Sadeghi was born and raised in Iran where he received his B.Sc. Degree in Chemical Engineering at the University of Tehran. He then pursued his Master's at Texas Tech where he discovered his passion for the linkage between Artificial Intelligence and Multidisciplinary Engineering. He is currently a senior Ph.D. candidate in the Abolhasani Lab at NC State University working on Smart Nano-manufacturing of Advanced Functional Materials Using Self-Driving Fluidic Laboratories.
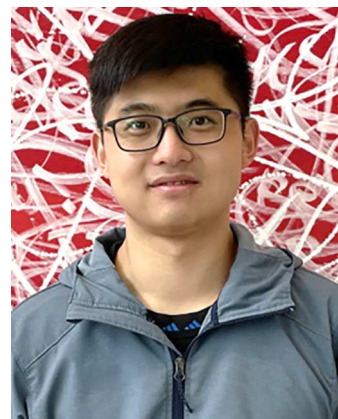

Richard B. Canty completed their doctorate in chemical engineering focusing on laboratory automation in ML-guided research platforms at the Massachusetts Institute of Technology in 2024. They are currently working as a postdoctoral researcher at the Abolhasani Lab at NC State University in Raleigh. Their research focuses on enabling robust automation via programmatic agency and the design of transferable automation solutions for laboratory research.

Nikolai Mukhin completed his B.Sc. degree in chemical engineering from the University of South Carolina in 2021, where he focused on

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Jinge Xu obtained his B.Sc. degree in Chemical Engineering at Xi'an Jiaotong University. He received his Master of Science in Chemical Engineering from the University of Washington, Seattle. He is currently a Ph.D. candidate in the Abolhasani Lab at NC State University. His research focuses on the data-driven synthesis science studies of colloidal QDs with autonomous robotic experimentation.

Fernando Delgado-Licona pursued his M.Sc.Eng. in the Decarbonization, Climate Change and Circular Economy group at Tecnologico de Monterrey in 2020, focusing on precision synthesis of metal oxides in flow. He is currently a Ph.D. candidate at NC State University in the Abolhasani Lab. Fernando is working at the intersection of process intensification and ML.

Milad Abolhasani is an ALCOA Professor and a University Faculty Scholar in the Department of Chemical and Biomolecular Engineering at NC State University. He received his Ph.D. from the University of Toronto in 2014. Prior to joining NC State University, he was an NSERC Postdoctoral Fellow in the Department of Chemical Engineering at the Massachusetts Institute of Technology (2014–2016). At NC State University, Dr. Abolhasani leads a diverse research group that studies SDLs tailored toward accelerated discovery, development, and manufacturing of advanced functional materials and molecules using fluidic microprocessors.

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