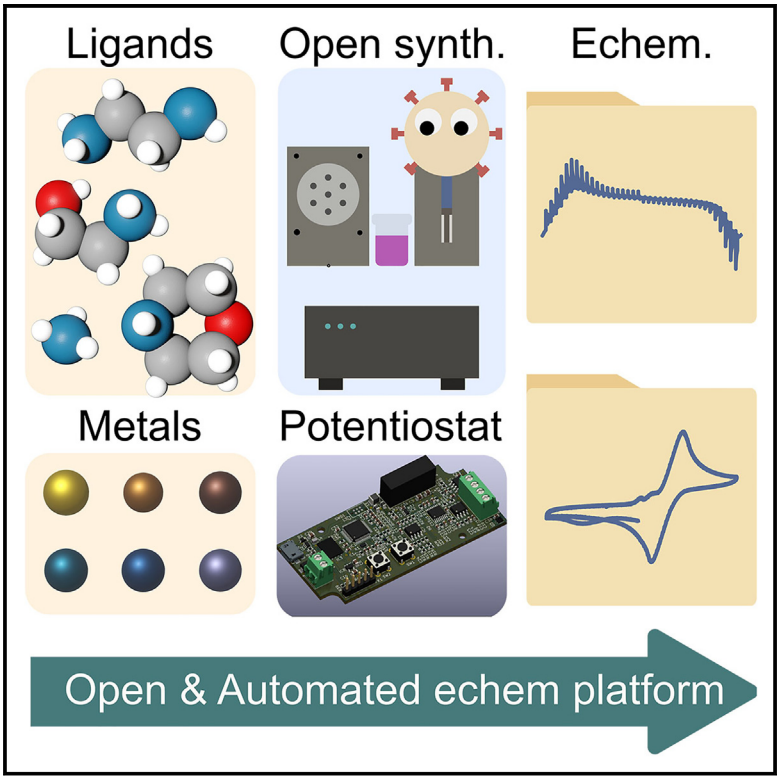
Device

Article

An affordable platform for automated synthesis and electrochemical characterization

Graphical abstract



Highlights

- Open-source, low-cost potentiostat for electrochemistry measurement
- Modular automation platform with online electrochemistry analysis
- High-level orchestration software for experiment process management
- Active decision-making and quality control

Authors

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In brief

This study presents an open-source, low-cost potentiostat integrated into a modular automated synthesis platform for high-throughput electrochemical analysis. Utilizing an orchestration platform, the system enables extensive control over experiments and active decision-making, demonstrating its capabilities through the generation of 400 electrochemical measurements automatically. By providing full transparency in design and software, this work aims to democratize the use of self-driving laboratories, promoting open science and enhancing reproducibility in electrochemistry research.

Develop
Prototype with demonstrated applications in relevant environment

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An affordable platform for automated synthesis and electrochemical characterization

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THE BIGGER PICTURE In recent years, self-driving laboratories (SDLs) have emerged as a powerful tool to expedite various areas of chemical research. For optimal functionality, these laboratories must be adaptable, readily modifying configurations to meet researchers' specific needs. Despite these advances, much of chemistry still depends on proprietary equipment from specialized vendors, which can be restrictive and difficult to customize for diverse lab setups. Moreover, ensuring reproducibility requires full disclosure of equipment details. In this work, we introduce an automated system featuring a cost-effective, self-designed potentiostat and a straightforward synthesis platform. We provide complete transparency by disclosing the electronic schematics of the potentiostat and the software used in the system. Our aim is to reduce the barriers to entry for SDLs and promote the principles of open science.

SUMMARY

Electrochemical techniques are pivotal for materials discovery and renewable energy; however, often the extensive chemical spaces to be explored require high-throughput experimentation to ensure timely results, which are costly for both instruments and materials/consumables. While self-driving laboratories (SDLs) promise efficient chemical exploration, most contemporary implementations demand significant time, economic investment, and expertise. This study introduces an open and cost-effective autonomous electrochemical setup comprising a synthesis platform and a custom-designed potentiostat device. We present an automated electrochemical module for SDLs that offers rapid deployment and extensive control over electrochemical experiments compared to commercial alternatives. Using ChemOS 2.0 for orchestration, we showcase our setup's capabilities through a campaign reacting different metal ions with ligands to form coordination compounds, yielding a database of 400 electrochemical measurements. Committed to open science, we provide the potentiostat design, campaign software, and raw data, aiming to democratize customized components in SDLs and ensure transparent data sharing and reproducibility.

INTRODUCTION

Self-driving laboratories[1–3] (SDLs) represent a paradigm shift in chemical research, integrating three key components[4]: (1) automated laboratory equipment,[5] (2) experimental planners,[6,7] and (3) orchestration software,[8,9] with seamless communication among these elements. Automated procedures enhance throughput and, once established, easily lend themselves to

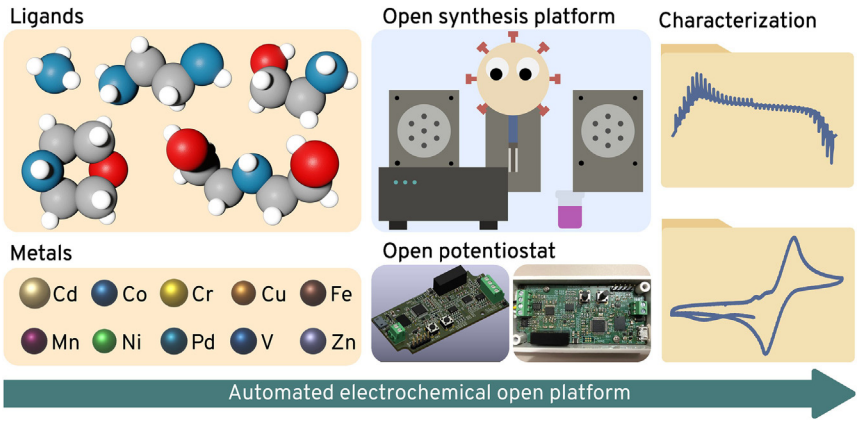

Figure 1. Schematic of this work
Given a set of ligands and metals, we mixed them using our open-synthesis platform "MEDUSA" and characterized them using our open-design potentiostat. Finally, the raw characterization data were stored in our database.

parallelization in a reproducible fashion, provided instrument choices and operational know-how are in place. While parallelization is well adapted to automated high-throughput calculations, device costs, access to reagents/consumables, and space limitations generally impede the broad application of parallelled automated experimentation. Recent initiatives within the open-source hardware and software community,[10] in tandem with the "maker movement,"[11] offer promising solutions, emphasizing customizability and cost effectiveness. The computer-driven, self-diagnosing nature of SDLs facilitates on-the-fly decision-making, potentially generating consistent and reproducible experimental data in both human- and machine-readable formats.[12–14]

In recent years, SDLs have found wide-ranging applications in materials discovery,[15–17] renewable energy production,[18,19] energy storage,[20] and synthetic chemistry.[21,22] High-throughput methodologies, particularly in materials synthesis and testing, have become pivotal, with electrochemical techniques playing a central role in characterizing candidate materials.[23] Importantly, electrochemistry SDLs have demonstrated their supremacy over traditional workflows in the pace and quality of generating electrochemistry data.[24–27] Nevertheless, most examples still rely on commercial potentiostats to carry out experiments, with applications that range from fundamental cyclic voltammetry (CV) to more advanced techniques.[28] Despite the common use of commercial potentiostats, their accessibility is hindered by their proprietary software, obfuscated data format, and, more importantly, the elevated financial cost that comes along with high-precision commercial platforms. Conventional single-channel desktop potentiostats are not designed for parallel analysis, facing challenges in high-throughput analyses, while multi-channel instruments compound expenses.

In response, the scientific community has endeavored to develop open-design potentiostat solutions since the early 1970s.[29–32] The more recent attempts aimed to further lower the economic barriers and enhance their compatibility with automated setups,[33–37] whereas some developed potentiostats focus on wireless capabilities, portability, and point-of-care applications.[38–40] All this progress was made possible by taking advantage of the improvements in electronic parts of potentiostats, such as microprocessors, analog-to-digital converters (ADCs), digital-to-analog converters (DACs), and operational amplifiers (Op-amps). Nevertheless, open-source devices that provide advanced functionalities inherent to their commercial counterparts and easy integration with orchestration frameworks are still lacking for SDLs.

Another crucial aspect of electrochemical SDL setups involves automated synthesis and sample transfer capabilities. While many commercial solutions are readily available, the advent of SDLs has sparked interest in open-source and cost-effective alternatives designed with modularity and adaptability in mind.[14] Although previous attempts have been made to integrate electrochemical systems with synthesis platforms, these solutions often tend to be confined to specific setups, missing the essential traits of generality and modularity. Previously, taking the advances in automating organic chemistry established by the Burke group[41] while further implementing modular design principles and open-source software, we introduced an extendable multipurpose platform, the modular, expandable discovery and understanding synthesis apparatus (MEDUSA), as the next generation of "The Machine."[7,42] Specifically, it has the full potential to incorporate both post-synthesis/-processing analyses in automation workflows and, therefore, is ideal for establishing end-to-end automated electrochemistry platforms.

This manuscript describes the development of a portable, open-source, and affordable semi-automated electrochemical module that can seamlessly integrate into any SDL setup.[7] Specifically, our module combines an in-house designed, compact potentiostat device with a basic version of the MEDUSA (Figure 1). The primary goal is to demonstrate the capabilities of this integrated setup by streamlining the generation of a comprehensive database containing metal/ligand complexes of electrochemical interest. The framework's affordability and open-source architecture make it an attractive option for electrochemical researchers seeking a flexible, cost-effective platform for high-throughput chemical screening. Integrating SDLs into advanced workflows can unleash end-to-end automation, facilitate high-throughput experimentation, and enable active decision-making, thereby producing high-quality datasets essential for both the experimental and machine learning communities.[43] This adaptability positions the framework as a valuable tool for generating reproducible and reliable data, with potential applications spanning redox flow batteries, environmental toxin detection, and beyond.

RESULTS

Potentiostat design and benchmarking

Potentiostats are essential characterization tools for electrochemical studies. However, most laboratories use potentiostats

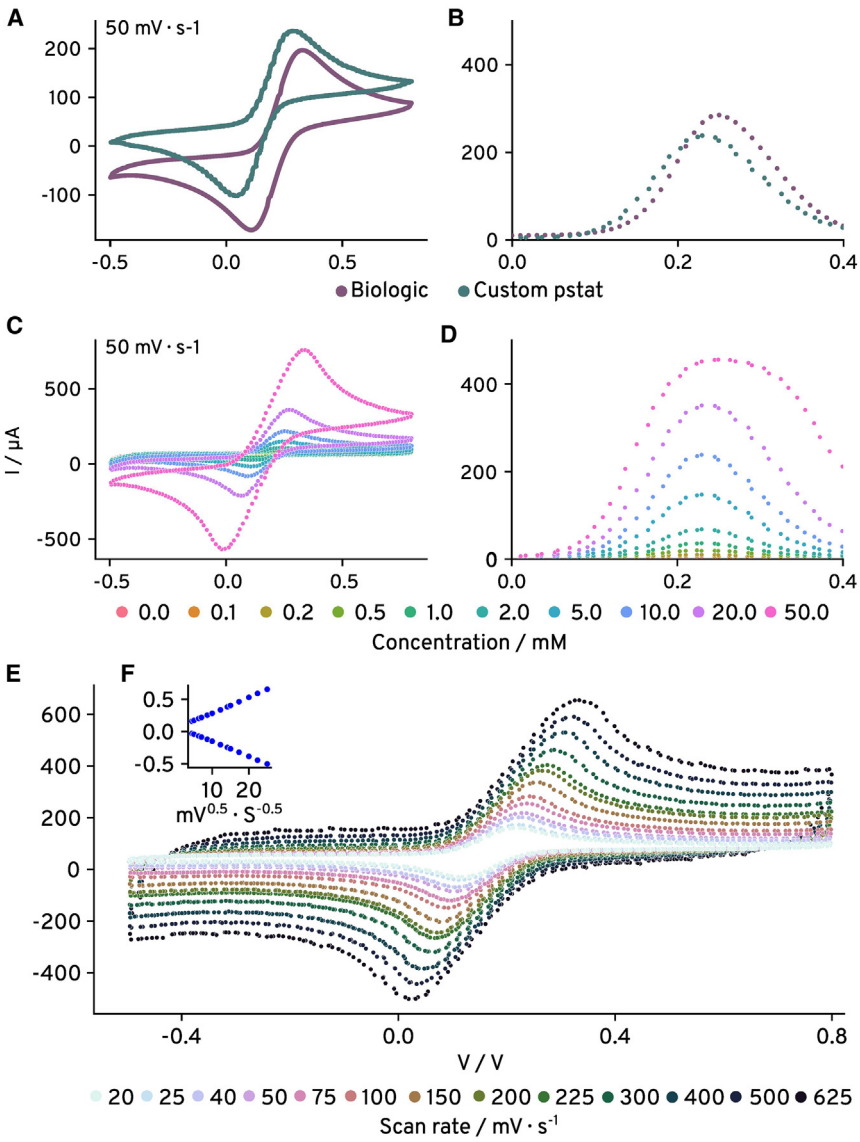

Figure 2. Benchmark of our custom potentiostat using $K_4[Fe(CN)_6]$ as reference and NaCl 1 M as electrolyte

(A and B) Comparison of CV (A) and DPV (B) techniques employing both a commercial potentiostat with a traditional setup (blue) and our custom platform (orange) at a reference concentration of 10 mM with a scan rate of 50 mV.

(C and D) Results of CV (C) and DPV (D) measurements at various reference concentrations using our custom platform.

(E and F) Characterization of the reference compound at different scan rates, maintaining a fixed reference concentration of 10 mM, utilizing our custom platform. Measurement parameters can be found in the electrochemical measurement section.

from commercial vendors that (1) are controlled by proprietary software, (2) use graphic user interfaces (GUIs), and (3) generate post-processing data. Because of these limitations, these potentiostats leave aside full control via an application programming interface (API) and direct access to raw measurements. While user friendly for manual operations, the three features mentioned above pose challenges when integrating into automated platforms, therefore calling for potentiostats well digitized to support data-rich experiments and electrochemical process analysis in modern SDLs. Applying the basic principles of electronics,[44] we have designed an open-source potentiostat using a STM32 chipset, together with open-source firmware and interface. Notably, the instrument benefits from its low cost (~120 CAD/device; see Note S1) and compact size (2 × 5 × 10 cm); consequently, it can be easily parallelized to enable high-throughput experiments (HTEs) even for groups with a limited budget or that are starting their first SDL setup. The potentiostat can be operated with a single USB cable for power and data transmission. The software design allows seamless implementation of highly customizable electrochemical protocols in addition to readily provided standard techniques. The detailed design of the potentiostat can be found attached as supplemental information. Figure S1 shows a three-dimensional (3D) render of the device. Note S2 contains a comprehensive description of the design and the firmware implementation.

In addition to low-cost potentiostats, the introduction of disposable printed electrodes and miniature flow cells has greatly changed electrochemical analysis, as it liberates human operators from tedious surface treatment of electrodes while significantly reducing material costs.[45–47] To demonstrate the capability of a low-cost electrochemistry platform, we benchmarked our homemade potentiostat against a commercial electrochemistry workstation (Biologic SP-300) using screen-printed electrodes (Dropsense; see the supplemental information for details). For both CV and differential pulse voltammetry (DPV) experiments with a 10 mM $K_4[Fe(CN)_6]$ standard solution, the performance of our low-cost platform and that of a traditional platform are comparable (Figures 2A and 2B). We further performed variable concentration experiments to investigate the sensitivities of our platform (Figures 2C and 2D), suggesting detection limits of 1 mM for CV and 0.1 mM for DPV techniques, which lay in the common range of both techniques. In variable scan rate experiments, a linear relationship could be identified between the peak current and the square root of the scan rate (Figures 2E and 2F), in line with expected diffusion-controlled redox events. In both variable concentration and scan rate experiments, the performance of our low-cost platform is competitive with the traditional platform based on a commercial potentiostat. Further benchmarks can be found in Figures S2–S5.

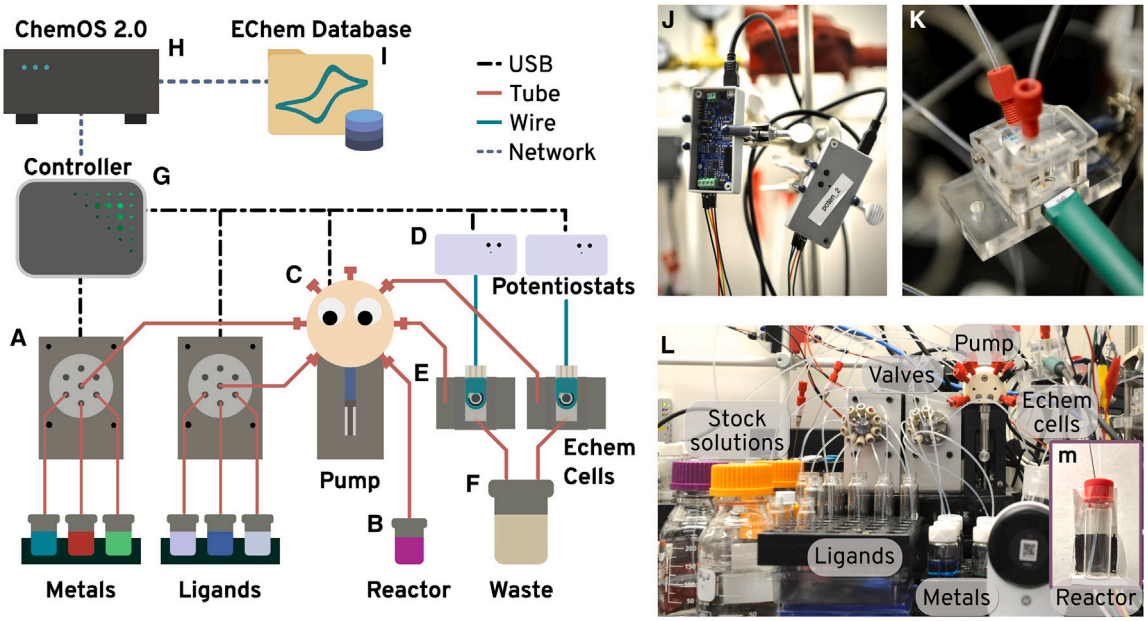

Figure 3. Platform design of automated complexation-electrochemistry platform

(A–I) Design of our framework divided into (A–C) automated synthetic platform (MEDUSA), (D–F) electrochemical setup, and (G–I) orchestration (J–L) actual experimental setups. The components are as follows: (A) selection valves, (B) chemical reactor, (C) syringe pump, (D) potentiostats, (E) electrochemistry cells, (F) waste, (G) driver controller, (H) orchestration software, and (I) database. The (solid) physical connections between the components are (red) tubes and (teal) wires, and the (discontinued) information transfer connections are (black) USB and (blue) network.

(J–L) Photos of the actual platform: (J) potentiostat devices, (K) Echem cell, and (L) the general setup.

Experimental setup

Our experimental setup, as illustrated in Figure 3, comprises an integrated framework for synthesis/characterization and orchestration components. In the synthesis component, we have two selection valves (Figure 3A), each linked to either metal or ligand solutions; a reactor (Figure 3B) designed to mix the metal and ligand candidates effectively; and a syringe pump (Figure 3C) connecting the aforementioned components to the electrochemical cells. The electrochemical setup consists of two potentiostats (Figure 3D), each individually connected to an independent printed electrode. These electrodes are housed within (Figure 3E) acrylic flow cells, connected to a waste vessel (Figure 3F). Coordination and control of these systems are orchestrated by a mini-PC (Figure 3G), which oversees and manages their operations, and a running SiLA2 server (Figure 3H), enabling the exposure of synthesis and characterization processes to ChemOS 2.0 (Figure 3I), facilitating remote automation and data collection. The raw data acquired from the potentiostat devices are collected by ChemOS 2.0, processed, and stored within an internal SQL database (Figure 3J) situated on an external device.

Semi-automated electrochemistry experimentation is made possible through an iterative workflow, as depicted in Figure 4. This workflow encompasses the following key steps: the pump transfers reference solution (10 mM $K_4[Fe(CN)_6]$, 1 M NaCl) to Echem cells (Figure 4A). The potentiostats conduct CV and DPV experiments, and results are processed on the edge (Figure 4B). The server actively decides on a continuing loop or human intervention notification based on processed data (Figure 4C). The pump transfers metal/ligand pairs with a specific ratio to the reactor for complexation (Figure 4D). The pump sends the reaction mixture to Echem cells (Figure 4E). The potentiostats conduct CV and DPV experiments (Figure 4F). Subsequently, cleaning is applied to eliminate any residual chemicals on the cell (Figure 4G). Finally, the server reports the results to the user (Figure 4H). The detailed complexation and electrochemical procedures are described in the experimental methodology section. While the coordination of ligands to metals involves various kinetic profiles and complicated thermal dynamic equilibriums, here we only measure the electrochemical profile of well-mixed reaction mixtures after staying at room temperature for ~5 min without extensively optimizing the reaction conditions and purifying the products.[48]

The raw and processed results generated in the steps in Figures 4B and 4F are promptly gathered and uploaded to ChemOS 2.0, where they are cataloged and stored within an SQL database (Note S3). Notably, as one pump serves two electrochemical cells/potentiostats (as seen in Figures 3D and 3E), once the step in Figure 4B concludes, the steps in Figures 4F and 4G are replicated in a second cell, albeit with a time gap due to the sequential operation of the pump. Given the limited lifespan of the printed electrodes (2–6 h of continuous operation), on-the-edge processed results of the reference measurement are chosen as approximates of the health of the electrodes. The server makes decisions on the processed data and prompts messages to a human chemist for intervention (see experimental methodology for details). Overall, the entire workflow is implemented as a Python script running on a computer hosting ChemOS 2.0 (Notes S4 and S5).

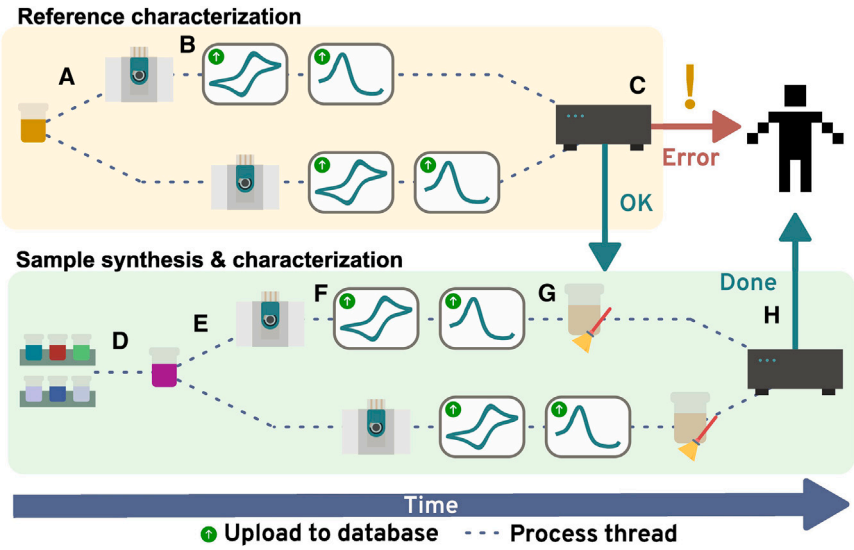

Figure 4. Iterative workflow for high-throughput experimentation

(A) Reference transfer.
(B) Reference measurement.
(C) Reference data processing and decision-making.
(D) Complexation reaction.
(E) Sample transfer.
(F) Sample measurement.
(G) Cleanup.
(H) Sample data processing.
Note that the blocks (yellow and green) represent different procedures using the same setup.

Data generation

The proposed workflow has been employed for synthesizing and characterizing ligand/metal complexes, involving the combination of 10 different metals and 10 distinct ligands in phase one of our campaign. This endeavor culminated in the generation of 100 unique complexes. The total lists of metals and ligands can be found in Tables S2 and S3, respectively. Each complex was prepared at 1:7 metal/ligand concentration ratios to ensure complete complexation, utilizing 1.0 M NaCl in water as the electrolyte/solvent and 1:1 HOAc/NaOAc as the buffer solution. Subsequently, comprehensive characterizations were conducted employing CV and DPV techniques. This thorough investigation resulted in a substantial database encompassing 400 voltammetry data. Noteworthy, the workflow embraces the potential to expand to a broader space, including additional ligands, different metal/ligand ratios, mixed ligands and additional orders, buffer pH, and reaction times.

To derive meaningful insights from the CV and DPV measurements, advanced data processing techniques were applied. For CV, a window average was utilized to rectify noisy data. In the case of DPV, the results were fitted to a Gaussian equation to enhance the signal's shape. Furthermore, a peak-finding algorithm, implemented in Scipy, was employed to identify the key peaks in both sets of measurements. To enhance the transparency, reproducibility, and overall clarity of our dataset, we have included both the raw and processed versions of the characterization measurements.

DISCUSSION

This section provides a comprehensive overview of the technical challenges, capabilities, and data management strategies associated with our framework for semi-automated electrochemical measurements. We begin by addressing key technical challenges encountered during the experiments, including electrode degradation and potentiostat controller issues. Next, we highlight the efficiency and adaptability of our autocomplexation and electrochemical measurement capabilities, showcasing the versatility of the MEDUSA system. We then discuss the role of active decision-making algorithms in enhancing the robustness of our setup. Following this, we delve into our data management strategy, emphasizing the importance of efficient data generation and management for ensuring reliability and reproducibility. Finally, we present a detailed analysis of the collected data, demonstrating the effectiveness of our approach in producing high-quality, reproducible results.

Technical challenges

Electrode degradation

While most parts of the experiments were performed without human intervention, the screen-printed electrodes degraded throughout the experiments, which is indicated by an increase of the voltammogram baseline and the diminishing of peaks corresponding to redox events (Figure S6). For reversible electrochemistry systems such as $K_4[Fe(CN)_6]$, the lifetime of a typical electrode could reach up to 12 h of operation. However, the lifetime may be significantly reduced due to irreversible processes (e.g., metal reduction and coating on the electrode) and heterogeneous samples (e.g., precipitation formation in reaction), which is exemplified by the electrochemical measurement of Pd complexes using $[PdCl_4]^{2-}$ starting material. In a typical example, one electrode can be used for 5–20 metal/ligand combinations. An estimation of the experimental cost can be found in Note S1.

Considering the electrode degradation varies across metal-ligand combinations, the degree of degradation cannot be guessed prior. To ensure the consistency and quality of our data, we used screen-printed electrodes that can be easily replaced and implemented two critical benchmarking criteria. In our experiments, each electrochemical measurement of an unknown sample started with a measurement of a known concentration of $K_4[Fe(CN)_6]$ solution (CV and DPV). The peak heights of both and the Gaussian fitting parameters (baseline, FWHM, etc.) of DPV were extracted. The results were benchmarked against the initial measurement and compared between parallel measurements from different cells, which provides information on electrode degradation. Such information was recorded for quality control and, more importantly, used

to actively inform and manage experiments (see active decision-making).

Furthermore, we realize that human-in-the-loop is essential for the quality control of experiments even with advanced decision-making algorithms.[42] In this case, the monitoring and evaluation of electrode degradation is the essential part of quality control, and we implemented a combined human-algorithm effort to provide solid realization of electrode degradation over experiment progress. Specifically, we pushed the post-processed data to human chemists through a slack bot (see computational tools) in human-readable formats, such as visualized voltammograms, and those chemists conducted quick sanity checks. Using this approach, we are able to execute clever experimentation with minimal human and instrument resources.

Potentiostat controller

During the experiment, several issues were identified: (!) while the synthesis platform was assembled by an undergraduate student in our research group within 2 h, it might be challenging for inexperienced researchers new to the system. We plan to prepare a protocol describing the assembly and usage of the platform in detail. (2) Potentiostats have a relatively high power draw of 600 mA each, which precluded the use of a Raspberry Pi 4 as the controller since they have has a power limit of 1.2 A. Although our decision was influenced by the immediate availability of a mini-PC, another option is to use the Pi 4 and connect a separate external power supply to the potentiostats to increase the number of supported devices. (3) The communication between the mini-PC and potentiostats is implemented using serial protocols without error detection, which occasionally leads to corrupt data. To improve reliability, we have included data verification using the Modbus protocol. However, Modbus was added at a late stage, so to ensure reproducibility, we made all the measurements with the firmware implementing the serial communication. Both firmware versions are available in our repository, although we recommend using the Modbus version for improved reliability.

Autocomplexation and electrochemical measurement capabilities

Despite the challenges previously described, our framework exhibited remarkable efficiency, executing 400 electrochemical measurements in a semi-automated mode. This achievement not only underscores the robustness of our approach but also highlights the promising potential of cost-effective setups for conducting diverse coordination chemistry and electrochemical experiments.

Integral to this adaptability is the modular architecture of MEDUSA, enhancing the overall extensibility of our system. This modularity facilitates ease of integration and positions our setup to navigate more complex electrochemical configurations, especially those necessitating multiple stations. Our autocomplexation capabilities not only meet the demands of conventional electrochemical techniques but also set the stage for exploration and innovation in more intricate electrochemical setups.

For example, while our focus is centered on CV and DPV, the potentiostat's adaptability allows for the utilization of dynamic voltage shapes (Note S1). For instance, a current hold function was easily implemented in the firmware, unlocking the chronopotentiometry (CP) analysis. Furthermore, advanced electrochemistry techniques, including AC voltammetry (ACV), squarewave voltammetry (SWV), and electrochemical impedance spectroscopy (EIS), are straightforward to implement using the potentiostat's Python interface without the need to modify the firmware.

Due to the scope of this work, our system has only been tested in ionic, high-conductivity environments, and its performance in different chemical settings remains to be evaluated. However, since both the firmware and schematics of the system are available, we anticipate that potential users will be able to implement their own functions and modify the electronics to suit the specific needs of their laboratories.

Active decision-making

Within our setup, alongside the firmware and automation code, a minimal but effective active decision-making algorithm (Figure 4) serves to alert users in case of reference measurement failures. Despite its simplicity, this feature enhances the robustness of our system by notifying users of potential issues promptly.

As we designed our framework, we identified diverse areas that stand to benefit significantly from the integration of active decision-making algorithms. These areas include tuning DPV parameters, dynamic characterization techniques, and intricate experimental planning targeting specific observables.[7] Incorporating such techniques would undoubtedly elevate our framework's quality and efficiency.

However, we acknowledge the inherent complexity of implementing these advanced decision-making algorithms, recognizing that their integration falls outside the current scope of our work. Yet, embracing our project's *libre* nature, we invite external researchers to explore and modify our existing setup and code. This collaborative approach encourages the implementation of these advanced features into diverse workflows, expanding the capabilities of our framework over time.

Data management

This robust and versatile setup is complemented by our data management strategy. Human operators, susceptible to stress and errors during repetitive tasks, pose challenges to the robustness of experimental campaigns, introducing uncertainties into measurements. Despite the initial investment in time and resources for our experimental setup, the enhanced reliability and robustness it brings significantly outweigh these costs. Automated logging capabilities within our setup play a crucial role. The data obtained are seamlessly stored and organized in an internal database, providing easy access and expediting the process of failure debugging. This not only ensures cleaner data management but also accelerates the identification and resolution of issues.

Our data management strategy integrates with ChemOS 2.0, serving as a centralized orchestrator. The SiLA2 server within our framework enhances reliability and simplifies data curation, embodying our commitment to human-readable and efficient experimental workflows. Key to this integration is using a JSON schema in the job file (Note S5), structured hierarchically to represent experimental variables. The SiLA2 server parses and translates this schema to the internal workflow operations, ensuring precise execution of experimental protocols.

Characterization results are presented in a universal CSV format, facilitating compatibility with various external data analysis tools. The coupling of job/result pairs with detailed logging information is systematically stored in the orchestrator's database. This structured approach allows for easy querying of experimental results, promoting accessibility and data-driven analysis. For a comprehensive understanding of the database schema, refer to Note S3.

Moreover, the low-level access to the code of both the autocomplexation platform and the potentiostat amplifies the benefits. The unprocessed data can be readily shared, fostering transparency and collaboration. Benefiting from this open approach, external researchers can detect errors, audit our code, and, in terms of Linus's law,[49] contribute to its continuous improvement over time. This collaborative cycle ensures not only precision and reliability in our data generation but also promotes the perpetual enhancement of the system's quality.

Data analysis

After the data collection, we proceeded to inspect the data thoroughly to ensure their reliability and reproducibility. Out of the 100 duplicates of CV experiments, only two pairs of voltammograms exhibit significant shape differences in terms of peak numbers and/or positions, while the same number of different pairs exists in the DPV experiments. Meanwhile, pairs exhibiting differences in peak intensities can be identified. These results suggest that our electrochemical measurement setup and activation decision-making algorithm can produce highly reliable and reproducible results, which could be challenging for manual systems. Noteworthy, although only 10 ligands and fixed conditions, including pH, metal/ligand ratios, and reaction time, were applied in our data collection campaign, we demonstrated that our approach is versatile enough to handle more complicated ligand space and varied complexation.

Among the successfully performed CV experiments, 16 examples do not show significant peaks corresponding to redox events within the measurement range (−1.2 to 1.1 V, electrochemical window of water). Similarly 24 DPV experiments do not show significant peaks in either cathodic or anodic scans, which contain all 16 of the aforementioned examples. These observations suggest that while they are a more sensitive technique in principle and as shown by benchmarking experiments with $K_4[Fe(CN)_6]$ reference solutions, DPV measurements with unoptimized parameters may not be sufficient for more general electrochemical measurements.

The peaks identified in DPV experiments tend to be more symmetric and less overlapping with each other compared to the CV experiments, making it easier to identify the peak positions and intensities for quantification purposes. However, DPV experiments take longer than CV experiments (253 vs. 115 s per experiment), even considering that 5 cycles were performed in all CV measurements. Additionally, the 16 examples show a reduction of signals with increasing CV cycle numbers, suggesting coating/deposition on the electrode surface, which leads to electrode degradation. These observations highlight the significance of optimizing electrochemical protocols to balance accuracy and efficiency in data collection.

Conclusions and outlook

We constructed an Echem semi-automated laboratory platform to unravel the synthesis and electrochemical measurements of metal complexes. Based on our homemade synthesis robot and potentiostat, as well as open-source software and hardware design, we provide a low-cost, accessible, and reliable solution for automating electrochemistry data acquisition. Empowered by ChemOS 2.0 and the active decision algorithm, we demonstrate the capabilities of our platform by creating a high-quality, reliable, open-source electrochemistry database containing 400 voltammograms at a speed and cost that can hardly be achieved by solely human operation.

We believe that this work can benefit data-rich research focusing on electrochemistry, and not only because of the impressive data volume, data consistency, and raw data accessibility. Importantly, this campaign is not limited locally. Instead the low-cost and open-source nature of our solution ensures a low-barrier knowledge transfer, therefore making it ideal to be delivered and implemented around the world. Additionally, the human-in-the-loop hybrid workflow offers dynamic potential, which is crucial for the reliability and productivity of SDLs, particularly those involving complex decision-making processes and limited initial knowledge. We envision that further adaptation of such a solution will finally lead to a delocalized and democratized electrochemistry self-driving lab community.

EXPERIMENTAL PROCEDURES

Experimental methodology

Experiment workflow

The complexation reactions were conducted on the MEDUSA, a robotic platform for automated chemistry synthesis. The platform is based on syringe pumps and selection valves and has a modular design for easy expansion and adaptation to downstream sample preparation and characterization.

In the context of this manuscript, two electrochemistry characterization modules, each containing an Echem flow cell and a potentiostat, were directly connected to the synthesis module, and all the syntheses and measurements were performed on a single platform automatically without human intervention except for refilling the stock solution and changing the electrodes.

Active quality control

The screen-printed electrode has a limited lifetime. To ensure the reliability and quality of data and avoid artifacts from surface degradation and/or coating on the electrode, we implemented an active decision-making strategy. We base this strategy on measurement and on-the-edge (controller device) analysis of the reference solution (10 mM $K_4[Fe(CN)_6]$, 1.0 M NaCl) and on-the-fly workflow management on the server.

The reference solution was transferred to the Echem cells, followed by DPV and CV measurements (see the electrochemical measurement subsection for parameters). An x64 mini-PC processes the DPV results as the edge device to generate the plot and corresponding Gaussian fitting, which are streamed to the server. Based on the stress testing, arbitrary thresholds of 0.20–0.25 V for the peak center (x0) and <0.1 V for deviation (σ) were chosen. Based on the established criteria, the server autonomously decides whether to continue or halt experiments. If an experiment is halted, then a notification is sent to a human chemist via a Slack bot (Note S6), prompting manual inspection and electrode replacement. To maintain consistency between duplicate cells and minimize the frequency of electrode changes, both electrodes are replaced even if only one fails to meet the criteria. Further details on the decision-making process are provided in Note S7, and the decision scripts are available in our Zenodo repository (https://doi.org/10.5281/zenodo.10633135).

Complexation reactions and clean-up metal-ligand complexation reactions were performed in the following manner.

(1) Add 0.25 mL of 1.0 M HOAc/NaOAc buffer solution.
(2) Add 0.75 mL of 3.0 M NaCl solution.
(3) Add 0.35 mL of 0.3 M ligand solution.
(4) Add 0.15 mL of 0.1 M metal solution.
(5) Purge 1.0 mL N_2 through the reaction mixture and then draw and dispense 1 mL of the reaction mixture; this step is repeated 3 times to ensure a good mix.

Cleanup was performed in the following manner.

(1) Pass 0.25 mL of water through each Echem cell 5 times.
(2) Fully empty the reaction vial and discard the residue reaction mixture to waste.
(3) Add 0.9 mL H_2O to the reaction vial and then discard the rinsing liquid to waste; repeat this step 3 times to ensure thorough cleaning of the reaction vial.

Electrochemical measurements

Both DPV and CV experiments were performed for the reference and reaction mixtures. Notably, to reduce the degradation of the electrode and avoid current spikes at the onset, DPV experiments were performed in one cycle, starting from an open-circuit potential (OCP) toward a minimum voltage (V_{min}), then raising to a maximum voltage (V_{max}), and finally returning to the OCP.

Two sets of parameters were chosen for the reference and reaction, respectively. The reference DPVs were measured in the range of −0.1 to 0.5 V at a 100 mV pulse voltage and 10 mV step voltage with a 50 ms pulse width and 500 ms period, and CVs were measured in −1.2 to 1.1 V for 3 cycles at 200 mV/s. The reaction mixture DPVs were measured in the range of −1.2 to 1.1 V at a 100 mV pulse voltage and 10 mV step voltage with a 50 ms pulse width and 500 ms period, and CVs were measured in −1.2 to 1.1 V for 5 cycles at 200 mV/s. Considering the short distance between electrodes and the relatively high conductivity of NaCl aqueous electrolyte solution, the iR drop in our measurement is expected to be low and was not considered.

Computational tools

The coordination and management of the experimental processes were executed using ChemOS 2.0,[8] which was integrated into the laboratory's local network. We employed an x64 mini-PC with the Debian Linux system and a virtual Python 3.11.2 environment to control the potentiostat, selection valves, and syringe. Communication between the controller and potentiostat was established through a serial communication protocol, aided by a Python interface built on top of Pyserial 3.5,[50] enhancing user interaction. In a similar fashion, we enabled communication between the selection valves and the syringe pump, utilizing MEDUSA drivers. Regarding the hardware connections, the valves, pumps, and potentiostats were directly connected to the USB ports of the PC. To ensure seamless recognition, udev rules were implemented to correctly identify the pumps and potentiostats. The Python interface of the potentiostat was designed with the capability to transmit target voltages in real-time or buffered mode. To create the voltage waveforms essential for CV and DPV measurements, we utilized Numpy 1.26.1[51] and Scipy 1.11.3.[52] Additionally, for data analysis, we employed pandas 2.1.1[53] and Matplotlib 3.8.0.[54]

For remote operation control, a SiLA2[55] server was deployed using the SiLA2 Python implementation 0.10.5. The client operates as a SystemD service and offers four distinct methods: (1) mixing the compounds and conveying them to the reactor, (2) performing CV, (3) executing DPV, and (4) cleaning. All methods accept input in the form of JSON with operation-related parameters. Methods 2 and 3 return measurement results in CSV format, while methods 1 and 4 return none. An error is reported in the case of a failure. To enable concurrent operations within the workflow, we leveraged the asyncio Python library. Before starting the orchestration with SiLA2, the robustness of the setup was tested by using simpler bash scripts running both potentiostats in parallel via subshells. The results of those tests have also been incorporated into the database. A Slack bot has been used to report the incidents and warnings regarding the process. The bot has been implemented sending requests via curl 7.88.1 to the rest API provided by Slack.

RESOURCE AVAILABILITY

Lead contact

Further information and requests for resources should be directed to and will be fulfilled by Han Hao (hann.hao@utoronto.ca).

Materials availability

This study did not generate new material.

Data and code availability

Potentiostat schematics, printed circuit board design (in Gerber format), bill of materials (in BOM file format), and the design file of the case are included in our Zenodo repository: https://doi.org/10.5281/zenodo.10633135. The current drivers of the potentiostat, as well as the Python interface to control it, can be found in our GitLab repository: https://gitlab.com/aspuru-guzik-group/potentiostat. The generated database, containing the raw and processed CV and DPV measured results of all the measurements, can be also found in our Zenodo data repository: https://doi.org/10.5281/zenodo.10633135. The processed data and voltammogram figures are uploaded as Data S1 and S2. MEDUSA drivers, potentiostat drivers/interface, and 3D printing design of potentiostat enclosures are available in our GitLab repository. Complexation robot controlling software is available in our GitLab repository: https://gitlab.com/aspuru-guzik-group/self-driving-lab/instruments/e_complex.

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AUTHOR CONTRIBUTIONS

S. P.-G. contributed to the methodology, writing of the first draft, firmware and software development, conceptualization, and supervision. A.G. contributed to hardware design and firmware development. G.D.A. contributed to firmware and software development and writing. M. Sim contributed to workflow development, orchestration, and writing. Y.C. contributed to the methodology, conceptualization, and editing. M. Somers contributed to preparation of experimental workflows and editing. C.H. contributed to firmware development. N.Y. contributed to experimentation and 3D design of the case. D.D. contributed to reviewing, editing, and funding acquisition. H.H. contributed to the methodology, writing of the first draft, data analysis, preparation of experimental workflows, conceptualization, and supervision. A.A.-G. contributed to conceptualization, funding acquisition, supervision, project administration, and writing review and editing.

DECLARATION OF INTERESTS

The authors declare no competing interests.

SUPPLEMENTAL INFORMATION

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