In the Mix: A workshop merging computational chemistry and electrochemistry alongside data science

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Abstract

As chemistry expands to more complex and interdisciplinary areas, a new generation of diverse researchers must engage with science and learn effective cross-disciplinary collaboration and communication. To these ends, we designed and implemented *In the Mix*, a graduate-student-led, two-day workshop for undergraduate students promoting collaborative science in the context of energy storage innovations. The interactive workshop was designed for future and emerging researchers to gain hands-on experience with data science, computational chemistry, and electrochemistry techniques that are critical in developing materials for battery technologies. Participants also toured commercial renewable energy facilities to help them connect discovery-based research with industry and broader societal considerations. The workshop content and structure ensured participants experienced the interrelatedness of the fields and understood the importance of collaborative research to yield scientific advances with real-world applications. An external team evaluated the workshop and participants' perceptions of their experiences. While our research context was energy storage, the workshop goals and outcomes are applicable to other contexts. Interdisciplinary, experiential workshops are a key avenue to broadening participation in science and research, and the ideas presented here can be readily modified for other scientific contexts and/or incorporated as broader impact activities.

Keywords: collaborative science, broadening participation, experiential learning, undergraduate and graduate education, redox flow batteries, electrochemistry, computational chemistry, machine learning

Introduction

Increasingly complex problems in science and engineering demand increasingly interdisciplinary solutions. Advances in science education research continue to revolutionize how post-secondary science, technology, engineering, and mathematics (STEM) students are trained, yet challenges in equipping students for the unique challenges of interdisciplinary collaboration remain. Thus, science educators must promote explicit collaborative experiences for emerging scientists.[1-10] Alongside the rich discipline-specific curricula, there is a growing need for more collaborative science education materials and greater prioritization of interdisciplinary and context-based training.[11-13] Such training experiences should also equip emerging scientists with relevant transferable skills, expand participation in scientific endeavors, and promote sustainable adoption of collaborative experiences. Indeed, funding agencies recognize this; a familiar example is the U.S. National Science Foundation's (NSF's) requirement for Broader Impacts in funding proposals.

As we seek to broaden participation in collaborative science,[14-19] we should implement equitable, evidence-based educational and research opportunities[20-22] while considering psychosocial factors.[23-25] Such initiatives often employ active learning, which both improves students' educational outcomes[26] and decreases equity gaps among minoritized student populations.[27] In fact, expanding access to evidence-based educational practices is a key objective called for by the U.S. National Academies of Sciences, Engineering, and Medicine (NASEM).[28] While a full review of impactful educational practices or active learning is beyond the scope of this paper, we note examples from two areas of active development. First, significant effort exists in the area of undergraduate research. This includes Course-based Undergraduate Research Experiences[29]

(CUREs), Group-led Undergraduate Research Programs (GURPs),[30] and experiences like NSF Research Experiences for Undergraduates (REUs).[31-33] Second, examples of efforts in undergraduate curriculum reform can be found outside of providing undergraduate research experiences.[7-9, 13, 34] These initiatives have documented success in improving student learning.

While CUREs and REUs offer significant benefits, these experiences are not accessible to all students. For example, a student may attend an institution that has no CUREs; REUs are only open to students who are U.S. citizens, nationals, or permanent residents;[32] and implementing a robust undergraduate research program can be expensive in time, money, and effort.[31] Furthermore, large-scale curriculum reform to emphasize context-based STEM education can be difficult.[7, 8] Thus, there remains a need for more accessible educational opportunities. Here, experiential workshops play a significant role. Hands-on workshops for high school students[35-42] and entering college students[43] have effectively engaged students with science and improved their perceptions of themselves as scientists. Many of these workshops have goals similar to CUREs,[29] but free, relatively short workshops provide substantial opportunities to broaden STEM participation. Moreover, workshops designed around a complex multidisciplinary problem can introduce more students to collaborative science.

We are engaged in collaborative science through the NSF-funded research project D^{3}TaLES (Data-enabled Discovery and Design to Transform Liquid-based Energy Storage),[44] which seeks to accelerate the development of materials for redox flow batteries (RFB).[45] A central challenge in designing materials for high-performing RFB is determining (or predicting) a molecule's reduction (oxidation) potential, which fundamentally limits maximum RFB voltage. However, structural changes to favorably tune reduction (oxidation) potential may unfavorably alter other molecular properties (e.g., solubility), producing a complex science and engineering problem requiring interdisciplinary solutions (SI Section 1). Within this context, we sought to prepare future researchers for collaborative science through a hands-on workshop based on the lessons learned through our own research.

Here we present *In the Mix*, a two-day experiential workshop promoting collaborative science, specifically in the context of energy storage. During *In the Mix*, students experience interconnected science by learning to predict and measure reduction potential throughout three modules: electrochemistry, computational chemistry, and data science. Module contents are interwoven and coalesce around the goal of finding better RFB materials, applying a research-based method of achieving durable learning known as interleaving.[46] The workshop also includes a beyond-the-university component shown to be important in other contexts.[41, 42, 47, 48] We implemented *In the Mix* twice, once in Kentucky in 2022 and once in Iowa in 2023. To evaluate the workshop, an external evaluation team administered participant assessment surveys before and after each workshop. Here, we demonstrate how such a research-focused outreach effort can both develop undergraduate students' research skills and connect them with collaborative science in a broad research context.

Methods

In the Mix goals

The graduate student activity leaders and project faculty used backward design to iteratively develop *In the Mix* by articulating the goals and desired outcomes, then designed the workshop accordingly.[49] The goals for this workshop were that undergraduate students:

- See themselves as scientists
- Gain experience working in team-based science
- Contribute to solving big, societally relevant problems
- Understand the value of and rationale for big data
- Acquire practical skills that equip them to contribute to ongoing research

Workshop structure

In the Mix occurs over two full days. The workshop consists of an introduction to energy storage (SI Section 1), three modules, and an external field trip. Each module highlights a scientific discipline relevant to energy storage research: experimental electrochemistry, computational chemistry, and data science (**Figure 1**). The external field trip showcases existing renewable energy technologies (e.g., solar, wind) that are currently limited by the lack of grid-scale energy storage. Together, these activities pair content knowledge and the development of research skills with immediate technological needs and societal motivation. These considerations are particularly important given the interconnectedness of motivation, perceived self-efficacy, and identity among students.[13, 20-22, 24, 25, 29, 30, 37-40, 42, 43, 50] We closed each workshop with a group dinner and a time for structured reflection on participants' and leaders' experiences.

Generic Schedule

In the Mix Day 1	
9:00	Welcome
9:15	Motivation & Background
9:45	Break/Transition
10:00	Computation, Part 1
11:00	Break/Transition
11:15	Data Science, Part 1
12:15	Lunch
1:00	External Field Trip
5:00	Finish Day
In the Mix Day 2	
9:00	Welcome
9:05	Experiment, Pre-lab
9:15	Experiment, Part 1
12:00	Lunch
1:15	Experiment, Part 2
2:15	Break/Transition
2:30	Computation, Part 2
3:30	Break/Transition
3:45	Data Science, Part 2
5:00	Finish Day

Figure 1. Schematics of *In the Mix*'s structure including a (left) summary of the three scientific disciplines highlighted in the workshop and (right) a general agenda for the two-day workshop.

Module contents

Each module includes an overview of the discipline and emphasizes its application to the search for redox-active materials for RFB. Specifically, each module relates the discipline to understanding candidate molecules' redox potentials. During the electrochemistry module based on the work of Ji et. al.,[51] students learn how reduction potential is determined experimentally through cyclic voltammetry (CV) as they perform CV measurements on several potential RFB molecules. Students then analyze their data to determine reduction potential along with other properties such as diffusion coefficient. In the computational module, students are introduced to computational chemistry and the basics of density functional theory (DFT) before learning how DFT can estimate reduction potential in a section adapted from an open-source workshop on reduction potential from MolSSI Education.[52] Students use DFT calculations to estimate the reduction potentials for the molecules used in the electrochemistry experiments and compare the results. In the data science module students are introduced to machine learning (ML) and then experience ML activities and their potential to rapidly predict properties like reduction potential.

Additional details concerning the workshop model content and construction are given in SI Section 2. The resources developed for this workshop use open-source and accessible software such as Google Collaboratory, and all materials including code notebooks, slide decks, and a sample schedule are available to the public for local implementations on GitHub.[53]

External field trips

A principal component of *In the Mix* is the external field trip, and the outcomes of the external field trip are multifaceted. First, the beyond-the-university experience connects the discovery-based research sampled during *In the Mix* modules with real-world applications. Visiting working renewable energy installations helps students understand the complexity of utility-scale energy and the many fields of expertise that are required to maintain and improve our energy systems. Second, visits to such renewable energy installations, i.e., a solar or wind farm, drive home the need for grid-scale energy storage innovations such as RFB. Understanding the scale of working utility operations makes the vast improvements needed in our energy storage systems tangible in a way that is not possible without the field trip. Third, the field trip helps to strengthen ties between academia and industry. Hearing directly from industry personnel and touring their operations gives students a window into the wide-ranging career possibilities in energy conversion and storage.

During *In the Mix 2022* in Kentucky, the group toured a local solar farm (**Figure 2**). This visit included a walking tour of the solar farm along with a discussion of the challenges and solutions in solar energy generation and maintenance. In particular, the facility managers described the challenge of storing solar energy from peak production in the afternoon for use during peak demand in the evening. We were shown the inside of an on-site 1 MW battery capable of storing up to 2 MWh that helped mitigate the challenge of mismatched production and demand.[54] In Iowa during *In the Mix 2023*, we toured a local wind farm. This visit began with a detailed discussion of wind power and the legal, logistic, economic, and engineering process of building new wind farms. We then toured the inside of a nearby wind turbine. As discussed in more detail below, these external field trips were the workshop highlight for most participants.

Figure 2. Photos from the external field trips to (top) a Kentucky solar farm in 2022 and (bottom) an Iowa wind farm in 2023. To get a sense of scale, note the people gathered around the base of the wind turbine in the lower right photo.

Implementation

In keeping with our goals to broaden participation in collaborative STEM, reduce barriers to participation, and provide an equitable opportunity to all participants, we did not charge a fee to attend the workshop, we provided meals to workshop participants, we offered free lodging to undergraduate participants, we provided transportation to the field trip sites, and in some cases, we provided transportation to the workshop itself. To promote the workshops, each year we created a workshop flyer with a QR code that linked to a Google Form for registration. Flyers were distributed widely within and beyond the institutions involved in D^3TaLES. Ultimately, the workshops successfully engaged a diverse group of students from various ethnicities, fields, and home institutions (SI section 3).

Results and Discussion

Workshop evaluation

A team of external evaluators invited all participants to complete online assessments both before and after each *In the Mix* implementation to assess participants' previous exposure to scientific research, their motivations for attending *In the Mix*, and their overall experience of *In the Mix*. Questions were designed to assess the efficacy of *In the Mix* and benefit the planning of future *In the Mix* workshops. Before survey collection, Institutional Review Board clearance was obtained through the University of Northern Iowa (approval number 21-0112). (For more information on evaluation methods, see SI Section 4.1.) In addition to demonstrating the outcomes of *In the Mix*, the external evaluation from the first year provided an opportunity to adjust and improve *In the Mix* when implementing the workshop the following year (SI Section 5).

Participants across both years of *In the Mix* generally had favorable impressions of the workshop: 9 (of 13) participants who completed the post-workshop questionnaire rated the workshop as excellent, 4 participants rated it as good, and no participants gave the workshop a fair or poor rating. When asked if they would recommend *In the Mix* to a friend or classmate, the vast majority (10 of 13) reported they would be very likely to recommend it. Additionally, all respondents reported improved research skills following the two-day workshop with 7 (of 13) reporting substantial improvement and 6 reporting a slight improvement. Eight (of 13) participants also described positive shifts in their understanding of connections among computational techniques, data science, and wet-lab (electrochemical) experiments in response to an open-ended question. One 2023 participant stated, "I am now able to make the connection that computational techniques can be used as precursors to wet labs." Students also reported increased understanding of the utility of big data in science, the value of transdisciplinary research,[55] and the connections between experiment, computation, and data science (SI section 4.2-4.4).

Generally, students' images of themselves as scientists also improved following *In the Mix* participation. While the sample size here is too small to support broad conclusions, quantitative data gathered indicate improvement in scientific identities[56] among participating students with the majority of students (8 of 11) reporting a self-image that is more aligned with that of a scientist following *In the Mix* participation (SI Section 4.2). Additionally, participant comments collected through both formal and informal feedback channels demonstrate students' improved conceptions of collaborative science and their places in it:

- *No matter what background you're from, you can have an impact on a project. (2023 participant)*
- *I learned how important collaborative work is. (2023 participant)*
- *I now understand a lot more about how computers can be used alongside lab work to make research more effective. (2022 participant)*

- *I learned to appreciate team science. There is no way I can know everything about science, but I can communicate with others. (2023 participant)*

While the workshop's primary goals were to expose students to interdisciplinary team-based science and improve their self-images as scientists, students also self-assessed their comprehensions of workshop material in the post-workshop survey. Asked to rate their understanding of concepts in each module after the workshop, the majority of participants reported understanding each activity at least somewhat. Self-assessed understanding was slightly higher for computational and experimental activities than for machine learning activities (SI section 4.5).

Finally, participants across both years most commonly found the field trip to be a highly rewarding aspect of the workshop; respondents specifically mentioned their interest in seeing direct, practical connections to workshop content. For example, one 2022 participant noted, "[The solar farm] was an impressive sight, learning about it was interesting, and it was very cool with how it directly connected to the python we learned earlier in the day." This suggests that the workshop successfully allowed students to see how research contributes to solving big, societally relevant problems. We recommend that future implementations of *In the Mix* include an external field trip to cement in students' minds the real-world applicability of the research and workshop materials. The field trip destination should leverage regional strengths in the discipline focus area of the workshop. Student participants were overwhelmingly local to the hosting institution, and their familiarity and connection to the region is an important aspect of connecting with the workshop objectives. Those seeking to implement collaborative science workshops in other research contexts could identify appropriate beyond-the-university field trips that directly tie workshop content to broader societal implications.

Graduate student leaders' experiences

While the primary objectives for *In the Mix* revolved around undergraduate experiences, *In the Mix* was valuable for graduate student leaders as well. Specifically, the workshop was designed and implemented by graduate students to improve their collaborative leadership and teaching skills (more details in SI Section 5). Ultimately, the collaborative leadership skills practiced in developing this workshop improved graduate students' abilities to contribute to their ongoing research, thus strengthening the collaborative research effort.

Hazards

Although quinones are generally safe, all participants and leaders should follow standard laboratory safety procedures during the electrochemistry module including handling chemicals with care and wearing appropriate personal protective equipment (PPE) such as goggles, gloves, and lab aprons/coats.[51] Additionally, during the external field trip, everyone should strictly follow any safety instructions given by the industry guide(s) such as wearing safety hats and staying together.

Limitations

The workshop's structure of two full consecutive days may be a participation barrier for students with less flexible schedules (e.g., students with full-time jobs). Though we increased participation during *In the Mix* 2023, the findings presented would be strengthened by more participants and additional workshop implementations. The pre- and post-workshop assessments were not mandatory and were not completed by all participants, therefore the findings do not necessarily represent the perspectives of all participants. Given the relatively small sample size for both workshop participation and completed assessments, we were unable to disaggregate the data based on race, ethnicity, or gender. Our workshop assessments focused on participant self-assessment of their learning. These assessments were not designed to directly and independently measure student learning, limiting the scope of assessment conclusions. Thus, further work is needed to validate educational outcomes. Our post-workshop assessment was administered shortly after each workshop; we did not attempt to measure any longer-term impacts among either participants or graduate student leaders. Longitudinal studies will strengthen future efforts to better understand the impacts of these activities.

Conclusions

Here, we describe an interactive and collaborative workshop, *In the Mix*, which was designed and led by graduate students for undergraduate student participants. The workshop employed active and experiential learning across three areas of science, with positive impacts on participants and leaders alike. Importantly, workshop participants enjoyed their experience, came to better understand the value of both transdisciplinary science and scientific big data, and improved their conceptions of themselves as scientists. While our research context was energy storage materials, the ideas presented here could be modified for a wide variety of scientific and engineering contexts. Our approach shows promise at scientific, educational, and ultimately societal levels.

Data Availability Statement

All workshop materials used for *In the Mix* are available at https://github.com/D3TaLES/In-The-Mix/. These are the updated versions of the materials that we used in the second iteration of the workshop in 2023. These include Google Collaboratory notebooks for Days 1 and 2 for both the Computational and Data Science modules as well as a procedure document and data analysis resources for the Experimental module. Additionally, for those wishing to adapt the workshop, this repository contains planning materials such as background/motivation slides, an example recruitment flyer, an example registration form, pre- and post-questionnaires for both participants and graduate student leaders, and a generic workshop agenda.

Associated Content

Supporting Information Document: Details regarding RFB and RFB materials; content of workshop modules and how the modules fit together; results and discussion of graduate student leaders' experiences; information on participant demographics; and a discussion of evaluation methods and additional details about evaluation results (PDF)

Workshop Materials: The zipped folder "InTheMix_GitHub" includes all materials hosted on the *In the Mix* GitHub repository. Note that Colab Python notebooks also exist in this folder as PDFs of the notebooks frozen after being run, showing all cells and cell outputs.

Author Contributions

R.D.: conceptualization, investigation, methodology, software, visualization, writing – original draft, writing – review & editing. **A.S.**: investigation, methodology, visualization, writing – original draft, writing – review & editing. **N.C.S.**: conceptualization, investigation, methodology. **R.O.**: methodology, writing – review & editing. **S.C.**: conceptualization, investigation, methodology, software, writing – original draft. **C.H.Y.**: conceptualization, investigation, methodology, software, writing – original draft. **H.J.Y.**: conceptualization, investigation, methodology, software, writing – original draft. **A.S.P.**: investigation, methodology. **L.G.**: investigation, formal analysis, visualization, writing – review & editing. **K.E.**: investigation, formal analysis, methodology, writing – original draft, writing – review & editing. **M.E.L.**: investigation, methodology, writing – review & editing. **B.G.**: conceptualization, funding acquisition, supervision. **S.E.M.**: funding acquisition, supervision, writing – review & editing. **S.S.**: conceptualization, funding acquisition, supervision. **S.K.S.**: conceptualization, funding acquisition, project administration, supervision, writing – review & editing. **C.R.**: conceptualization, funding acquisition, project administration, writing – review & editing. **J.L.J.**: conceptualization, funding acquisition, methodology, project administration, resources, supervision, writing – review & editing. **C.M.T.**: conceptualization, funding acquisition, methodology, project administration, supervision, writing – original draft, writing – review & editing.

Acknowledgments

This work was generously supported by the National Science Foundation (NSF) under Cooperative Agreement Number 2019574. We thank Cornell College for assistance with travel funding, and we are grateful for the use of facilities at Eastern Kentucky University and the facilities and laboratory staff at the University of Iowa. We wholeheartedly thank the entire D^{3}TaLES (https://d3tales.as.uky.edu/) team for their insights into the development of this workshop. Specifically, we thank Vinayak Bhat, Parker Sornberger, Jordan Chelle, Sashen Ruhunage, Darby Duffy, Chamini Perera, Balaji Sesha Sarath Pokuri, and Kieran Luedke. We would also like to thank Mr. Aron Patrick and his team at PPL Corporation for their time to provide a tour of the solar facility of the E.W. Brown Generating Station in Mercer County, Kentucky, and Mr. Alan Arnold and his team at Alliant Energy for their time to provide a tour of the English Farms Wind Farm operations center and wind turbine in Poweshiek County, Iowa. Finally, we remember and celebrate the ways Dr. Susan A. Odom helped so many come to see themselves as scientists. Dr. Odom saw and affirmed potential long before people were able to see it in themselves, and she eagerly and generously welcomed new researchers to the team. Though Dr. Odom never got to see this initiative realized, her legacy lives on through *In the Mix*.

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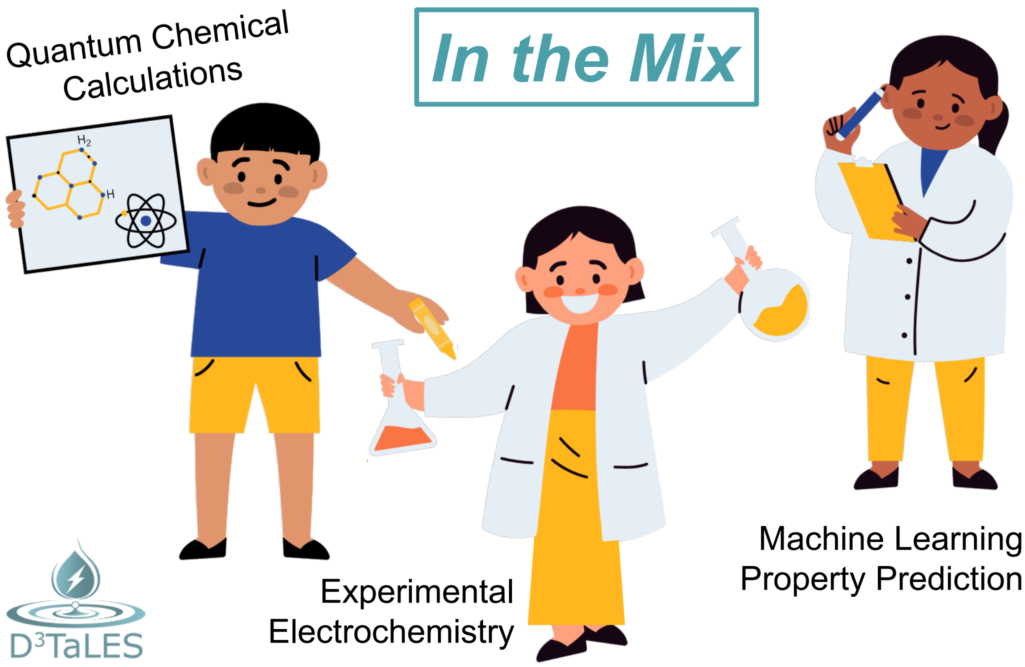

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