CHEMICAL SCIENCES ROUNDTABLE

BREAKOUT SESSION 1

Out of the Box: Providing the Tools and Resources Needed to Prepare Undergraduates for Automation

Date: November 16, 2021
Time: 1:45-3:30pm

Team:
Arsalan Mirjafari, Florida Gulf Coast University (facilitator)
Martin Burke, University of Illinois at Urbana-Champaign
Timothy Jamison, Massachusetts Institute of Technology
Rachel Switzky, University of Illinois at Urbana-Champaign
Saad Shehab, University of Illinois at Urbana-Champaign

ABSTRACT
This initiative aims to prepare chemistry undergraduate students for the future of synthetic chemistry by providing a robotic platform to optimize reaction conditions or screen catalysts. The goal is to close the skill gap between academic training at the undergraduate level and automated synthetic approaches common in the chemical industry. We intend to develop a low-cost (*i.e.* $999.99) viable automation technology with the ultimate goal of widespread dissemination to every teaching lab, primarily in resource-limited institutions.

SESSION GOALS
Identify learning objectives and resources necessary for introducing undergraduates to automation in chemistry. The goals will be achieved through an exercise of designing and filling a "box" with tools, concepts, and resources. These boxes should have the capacity to be delivered to undergraduate institutions, containing all the necessary elements to conduct an automation experiment and/or provide an automation "experience."

Timing	Activity
1:45-1:50pm	**Introduction**
1:50-2:20pm	**Activity I. Ideate: how do we introduce automation to the classroom?** Participants will utilize their workshop materials while working in groups with other participants to understand how we might best introduce automation concepts to undergraduate students in order to inspire future innovation and application of chemistry automation.
2:20-2:45pm	**Shareback and Discussion** Participants will share what they uncovered through discussion and exploration with their groups to the rest of the breakout session participants.
2:45-3:15pm	**Activity II. Brainstorm: what should go into the ideal box?** Participants will work with their groups to ideate around what would go in their ideal kit based on outcomes. Each group will create a low fidelity prototype to represent their kit and develop a budget for the potential cost for the kit.

3:15-3:30pm	**Shareback and Discussion** All participant groups will present their kits. Each team will have 2 minutes.

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Breakout Session 2

Graduate Education – Create an on-line textbook to serve as a resource for an upper-level class or for students and researches seeking to gain a broad introduction to automated and accelerated chemistry.

Date: November 16th, 2021
Time: 1:45pm-3:30pm

Facilitators:
Anne LaPointe, Cornell University
Nicola Pohl, Indiana University

ABSTRACT
This initiative aims to develop an online textbook that provides an introduction to all aspects of automated and accelerated chemistry (AAC). The course materials will be primarily geared towards graduate students and researchers who wish to learn about the concepts and strategies used in modern accelerated chemistry, and will also be adaptable for use in an upper level undergraduate course.

Workshop Goals: Identify learning objectives and then "design" an open source textbook for graduates and postgraduates that could serve as the basis for a one semester class or self-taught modules on topics such as experiment design, screening strategies, automation types and sources, illustrative case studies and an appendix of useful resources

Timing	Activity
1:45-2:00 pm	**Introduction to workshop** An introductory presentation will be given to set the context for the discussion. Participants will be given a copy of the tentative working outline.
2:00-2:20 pm	**Discussion of existing coursework/resources and learning goals for online textbook** Participants discuss their experiences teaching automated and accelerated chemistry and whether they have any course materials already developed. Overarching learning objectives for the online textbook will be identified.
2:20-2:40 pm	**Designing the open source textbook (all participants)** For each section, participants will brainstorm on content and organization, fine-tune the working outline and define specific learning objectives for each section and subunit. Participants will select the section that they are most interested in.
2:20-2:45 pm	**Part 1: Concepts, definitions and methods (all participants)**
2:45-3:15 pm	**Breakout session A: Logistics, instrumentation, and unit ops**
2:45-3:15 pm	**Breakout session B: Case studies and appendix/resources**

3:15-3:30 pm	**Participants finalize outline, volunteer to create content, and set timeline.**

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Breakout Session 3

Advancing automation and beyond -- creating a blueprint for a collaborative initiative

Date: November 16th, 2021
Time: 1:45 pm-3:30pm

Facilitator:
Shane Krska, Merck Research Laboratories

ABSTRACT
This session aims to gather diverse stakeholders from academia, industry and funding agencies to define and discuss the characteristics of a consortium that would "democratize" chemistry automation. Existing initiatives will be identified and their strengths and limitations will also be discussed. The goal is create a consortia that works towards creating an inclusive system to advance the utilization of automated chemistry across undergraduate and graduate education.

Workshop Goals: Brainstorm possible structures (organizational, legal) that could provide a framework to enable effective cross-collaboration between industry and academia.

Timing	Activity
1:45-1:55	**Goals and Overview.** Instructions for break-out sessions will be given.
1:55-2:10	**Activity I. Identifying the problem statement: What avenues of laboratory automation should the consortium focus on? (~15 min.)** Participants will begin the activity by reviewing the straw man proposal. Next, they will explore the intersection between industry and academia and identify the key questions that should be addressed to understand the value of automation. Guiding questions: *What value does automation bring to industry? How does academia envision using automation? How could these efforts be designed to serve the broader purpose of increasing diversity, equity and representation in the chemical sciences?*
2:10-2:15	**Virtual Report Out**
2:15-2:30	**Activity II. Gap analysis and mapping to resources and capabilities: What are the roadblocks to the democratization challenge? (~15 min.)** Group will work together to identify current and potential challenges involved in connecting industry with academia using laboratory automation. Guiding questions: *What resources do both industrial and academic researchers possess that could be employed to address these gaps? What is the potential role of federal funding? What are some current and available resources (i.e. software)? What are ways that industrial and academic researchers could collaborate and employ their resources together to increase access automation training? What are the cybersecurity concerns?*
2:30-2:35	**Virtual Report Out**
2:35-2:40	**5 minute break**

2:40-2:55	**Activity III. Potential collaboration frameworks: How do we bridge the gap and who wants to be involved?** Participants will work with their groups to discuss the different collaboration framework. Guiding questions: *What sorts of structures (organizational, legal) could provide a framework in which these industrial/academic collaborations could thrive? What are the inherent strengths and weaknesses of each of these collaboration models? What are the next steps? Who wants to be involved in further discussions? Who else should we reach out to?*
2:55-3:00	**Virtual Report Out**
3:00-3:30	**Group Discussion**