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Data driven acceleration of materials discovery and upscaling through correlative spectroscopy and lab-scale manufacturing

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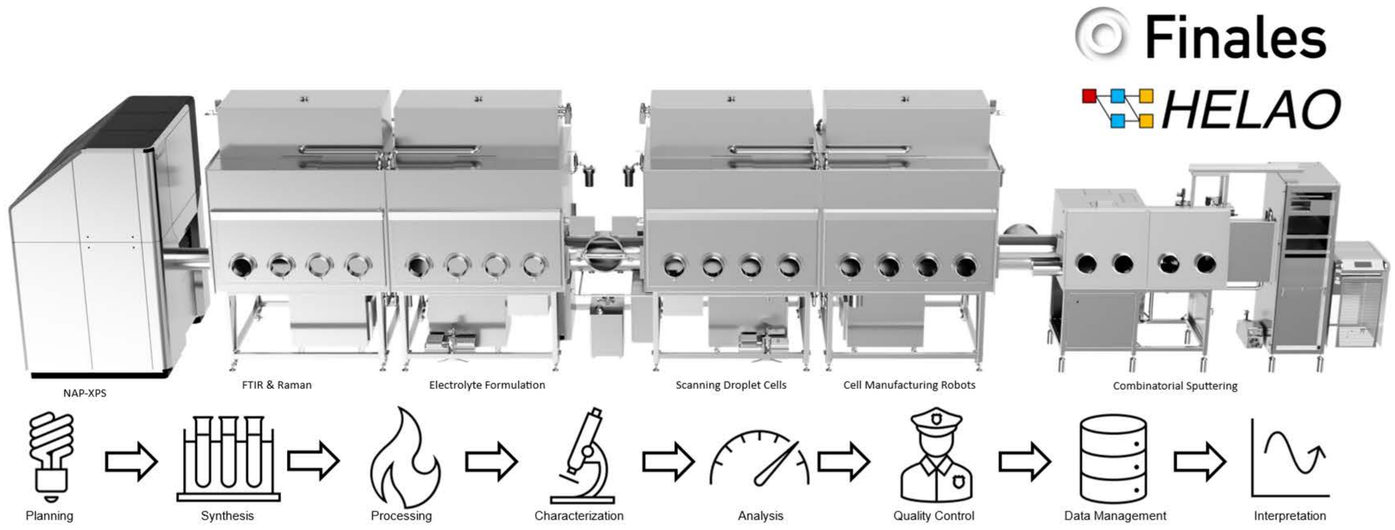
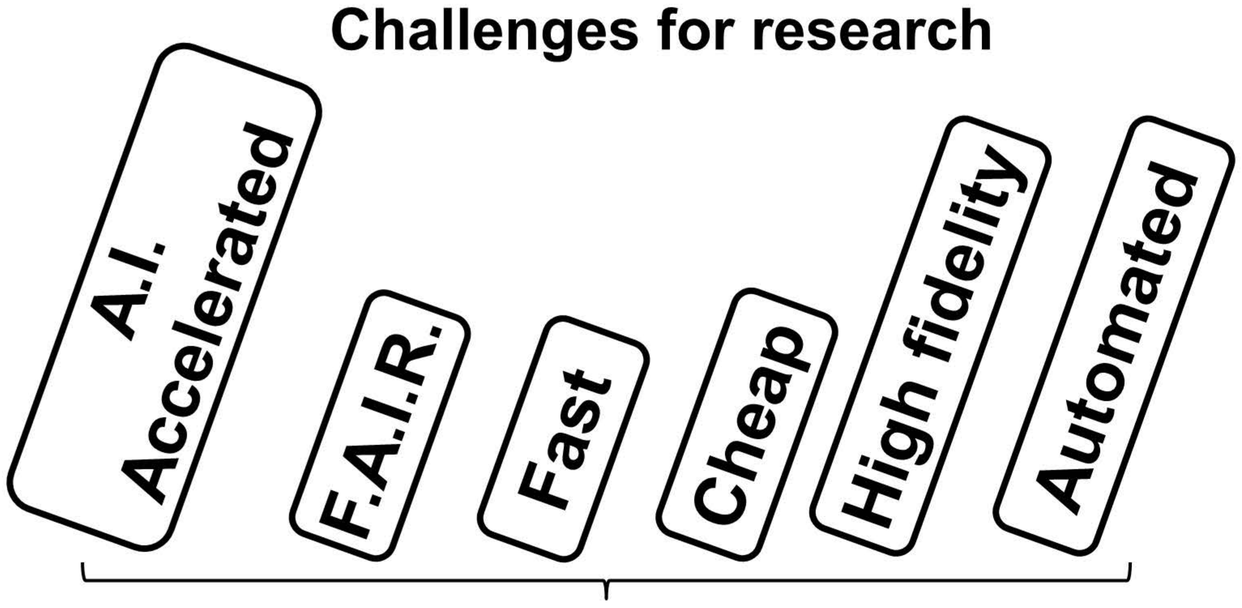
- Short and long-term storage of intermittently available renewable energy nessitates batteries and catalysis
- New and improved sustainable materials are needed ASAP
- Integration of automated experiments and data science is a viable route for acceleration
- Challenges in automation are solved by modern framework



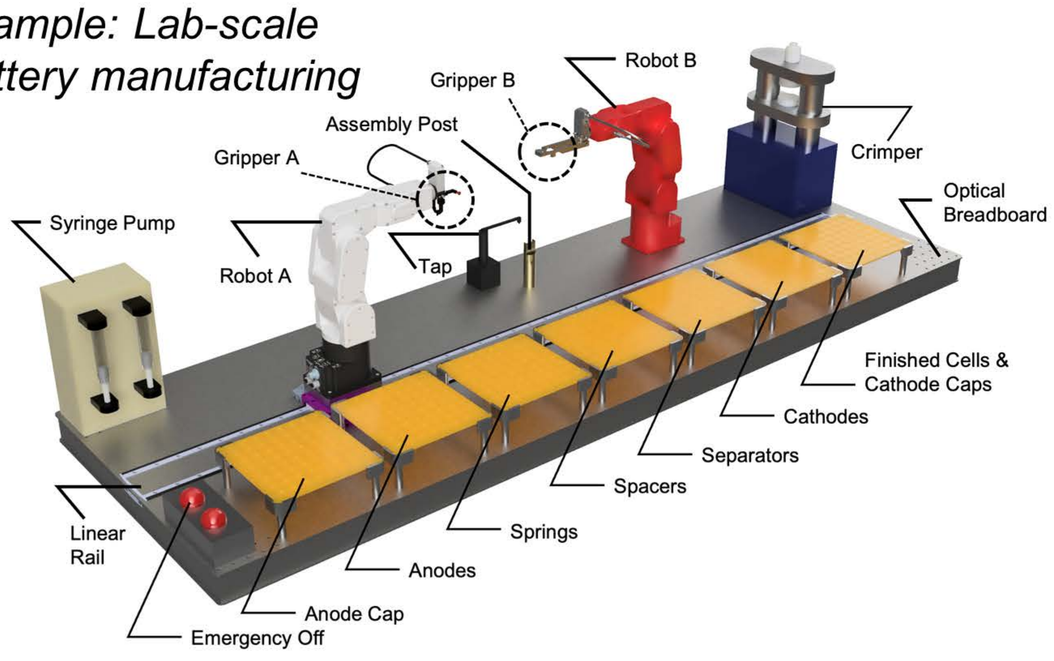
Challenges for research



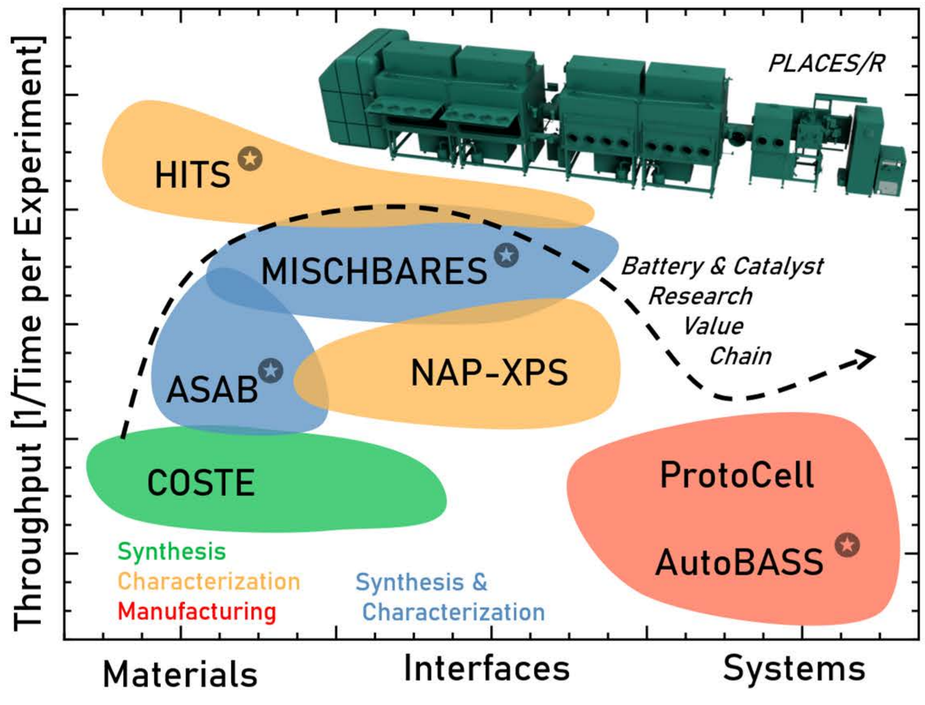
- If we want to go from the milimeter to the meter and from the mW to the GWh scale we need a new paradigm for conducting research
- Materials acceleration platforms offer such a paradigm shift in which automated instruments are integrated with AI
- Overall this reduces the time and cost per experiment also for high-fidelity measurements
- Data management is key to the overall sucess as well as the availability of well documented APIs for instruments and laboratories

Can we have all of this for energy storage research?

Example: Lab-scale Battery manufacturing



Yes, if we integrate automated research instruments with AI and data management



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1.Stein, H. S. & Gregoire, J. M. Progress and prospects for accelerating materials science with automated and autonomous workflows. *Chem. Sci.* (2019).
2.Stein, H. S. *et al.* From materials discovery to system optimization by integrating combinatorial electrochemistry and data science. *Curr. Opin. Electrochem.* 101053 (2022).
3.Stein, H. S. Advancing data-driven chemistry by beating benchmarks. *Trends Chem.* (2022).
4.Rahmanian, F. *et al.* Enabling Modular Autonomous Feedback-Loops in Materials Science through Hierarchical Experimental Laboratory Automation and Orchestration. *Adv. Mater. Interfaces* **9**, 2101987 (2022).
5.Zhang, B., Fischer, L., Sanin, A. & Stein, H. S. Robotic cell assembly to accelerate battery research. *chemRxiv* (2022) accepted in Digital Discovery