

## Machine learning aided, closed-loop optimization of electrodeposition processes in a Material Acceleration Platform

**Mert Ozan**, Annica Heyne, Ahmad Rashid Hazem, Matthias Dimper, Ozlem Ozcan  
Federal Institute for Materials Research and Testing (BAM)  
Unter den Eichen 87 12205 Berlin, Germany  
[mert.ozan@bam.de](mailto:mert.ozan@bam.de)

The progress in the automation of experimentation has picked up pace, facilitated through the development of autonomous agents such as Self-driving Labs (SDLs) and Material Acceleration Platforms (MAPs) [1, 2]. The quintessence of MAPs is in the reproducibility of the experimentation and data analysis which enables effective learning and closed-loop optimization using the high-quality data and metadata. Achieving this requires careful design of workflows combining different modular hardware and software components. In the context of advanced materials, MAPs have the potential to accelerate the discovery process by at least an order of magnitude.

We have developed a MAP (Figure 1) tailored for metal electrodeposition and corrosion research (Figure 1). The system integrates various instruments, including pumps and valves for liquid handling and a scanning electrochemistry setup, coordinated through a Python-based backend. The test cell can run up to four cells simultaneously allowing efficient reproducibility checks. Open circuit potential monitoring (OCP), electrochemical impedance spectroscopy (EIS), linear polarization resistance (LPR) chronopotentiometry (CP) and chronoamperometry (CA) are preconfigured in the backend and can be combined into flexible sequences by the user.

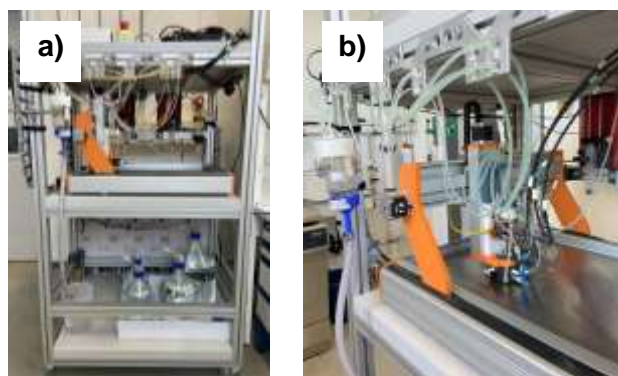
Achieving full autonomy requires fail-proof hardware and an efficient machine learning (ML)-driven design of experiments. We have tackled the former by an iterative design of the electrochemical cell and introducing reproducibility and quality checks during the data collection and evaluation. The MAP workflow was demonstrated with a case study on the optimization of the corrosion properties of electrodeposited Ni-alloy thin films on carbon steel substrate. Optimization is performed using Bayesian Optimization (BO) due to its rapid convergence, leveraging both the mean and variance of the data. Additionally, the results of the optimization campaigns are compared with other ML algorithms to evaluate their respective capabilities. Comparison of the optimization data across different algorithms highlights the importance of method selection in ML, as some models are more suitable for a particular system than others and cannot be generalized.

Overall, our work demonstrates the successful implementation of artificial intelligence in the discovery of advanced materials. The presentation will summarize the design and build phase of the electrochemical MAP, our data clearance and verification process and the results of the case study with a special focus on the comparative evaluation of different ML algorithms in terms of their effectiveness.

## References

- [1] Tom G, et al. Self-Driving Laboratories for Chemistry and Materials Science. *Chem Rev.* 2024;124(16):9633-9732. doi:10.1021/acs.chemrev.4c00055
- [2] Stier SP, et al. Materials Acceleration Platforms (MAPs): accelerating materials research and development to meet urgent societal challenges. *Adv Mater.* 2024;36:2407791. doi:10.1002/adma.202407791

## Figures



**Figure 1.** **a)** The MAP consists of three levels. The bottom level stores the electrolytes with their pumps and waste management. The mid-level houses the experimentation area where the XYZ-Gantry and the electrochemical cell is located. The top level contains electronic hardware, such as controllers, power supplies and potentiostats, etc. **b)** Snapshot image during the electrodeposition in the optimization campaign.