Guiding experimentalists with machine learning towards optimal Ni-W coatings for fuel cells

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The need to reduce our dependence on fossil fuels with the help of green energy and the development of efficient solutions for energy storage are among the most urgent challenges of current times. In this context, hydrogen technology emerges as a key factor, offering a clean fuel with a high energy density which can be produced through water electrolysis. However, the widespread usage of hydrogen as an energy vector is hindered by a significant bottleneck, namely, most electrodes contain platinum group metals (PGMs) due to their high catalytic activity and stability. Such PGMs are scarce and costly and prevent the use of hydrogen and fuel cells on a larger scale. In this context, the NICKEFFECT project[1] aims to develop novel Ni-based coating materials to replace PGMs and ensure high efficiency in key applications such as fuel cells.

In this work, Ni-W films have been electrodeposited in acidic medium and the performances of these films have been optimized through an active learning methodology depicted in Figure 1. The 24 sets of deposition parameters that were initially sampled experimentally were used together with the measured catalytic activity to train a simple model based on random forests. After only two rounds of active learning, each suggesting batches of 10-20 new deposition parameters, the performances reached by suggested samples overperform those obtained previously. This work shows that it is possible to make use of machine learning to guide experimentalists towards an optimal solution even when the amount of experimental data is limited.

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References

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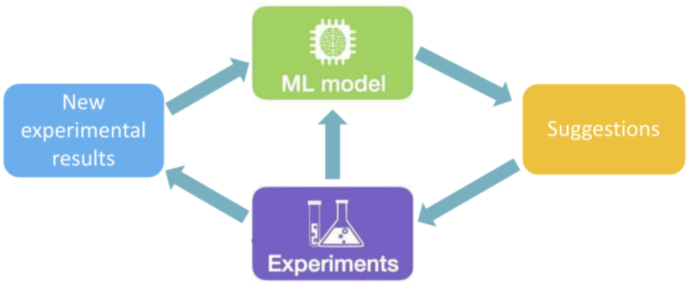

Figure 1. Active learning loop for optimizing experimental setups.