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Towards the automatization of catalysts synthesis thanks to real-time *in-situ* Raman spectroscopy coupled with artificial intelligence

This project aims to automate the synthesis of compounds of interest through interoperability between synthesis and characterization tools, with control based on machine learning models. The goal is to explore the feasibility of this approach on a simple reaction system, based on the controlled addition of an acid to a precursor (Na2MoO4, K2WO4, Na3VO4), to study and control product formation under dynamic conditions. An innovative reactor was developed to enable real-time monitoring of the reaction, including pH, temperature or conductivity probes and a Raman spectrometer[1]. The spectral data collected is used to train machine learning algorithms, including unsupervised (PCA, clustering) and supervised (regression, classification) approaches, as proposed in recent work on chemical process optimization[2]. These algorithms are used to predict and optimize synthesis conditions by identifying influential parameters. Figure 1 illustrates the overall workflow, including synthesis automatization, real-time monitoring via Raman spectroscopy, and analysis by machine learning models, all connected by a feedback loop to dynamically adjust experimental conditions. Initial results confirm the feasibility and effectiveness of this integrated approach, clearing the way for intelligent, continuous optimization of synthesis processes.

Figure

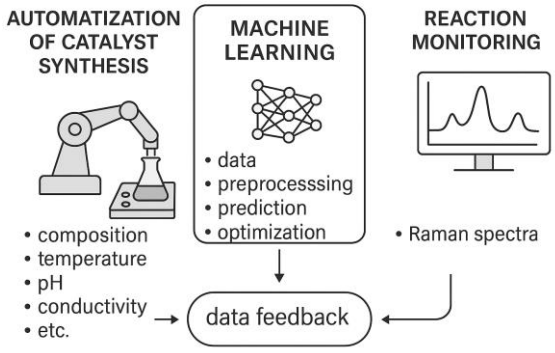

Figure 1: Workflow diagram for machine learning-assisted catalyst synthesis

References

[1] Y. Zheng, X. Wang, Z. Wu, *Industrial & engineering chemistry research* (2022), *61*, 5578-5592.
[2] A. Angulo, L. K. Yang, E. S. Aydil, M. A. Modestino, *Digital Discovery* (2022), *1*, 35-44.