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Quantum Active Learning for Materials and Homogeneous Catalysis Design

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Artificial intelligence (**AI**) has already met quantum computing[1]. This is explored here through the development of a *quantum active learning*[1] (**QAL**) method for quantum design of experiments (**QDOE**). QAL uses quantum machine learning (**QML**) regressions and their uncertainties for decision making (the agent), Fig. 1-left. QAL and classical AL (**AL**) are implemented in the MLChem4D[2] software. MLChem4D was used for QDOE of two problems using QAL: **(i)** perovskites optimization (e.g. band-gap minimization); **(ii)** reactions yield maximization of catalytic oxidation of β-citronellol with dioxygen[3]. Fig. 1-center shows the QAL results for double-perovskites band-gap minimization using quantum support vector regression (**QSVR**), compared to classical SVR. QAL with different feature maps – to build QSVR models with fidelity quantum kernel – performed better than the classical **AL** – using classical **SVR**[2], with radial basis function kernel[2]. For homogeneous catalysis reaction (Fig. 1-right), QAL and classical AL were employed using classical Gaussian process (GP), SVR and QSVR with different feature maps. Note that the reactions conditions search using QAL and AL have similar performance and the optimum reaction condition is: yield equal to 99 % when [Pd] (catalyst) = 0.01 M; [BQ] (electron transfer mediator) = 0.10 M; P = 10 atm; T = 80 °C and time = 7 hours. This result was confirmed experimentally.

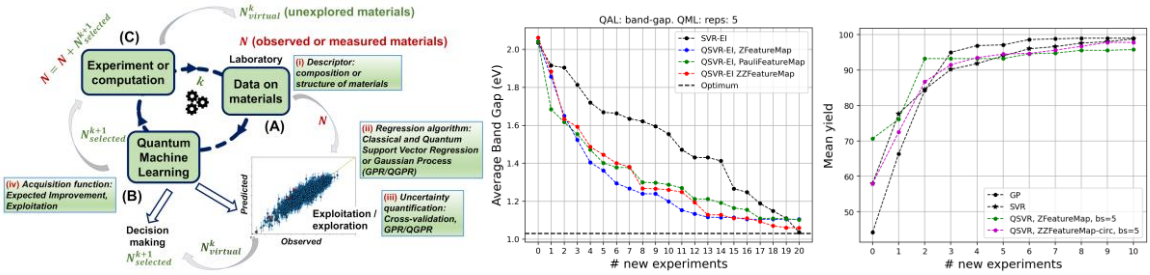

Figure 1. Left: *QAL and AL methods.* ***Center:*** *average $AA'BB'O_6$ (double-perovskite) band-gap minimization for 20 QAL independent runs.* ***Right:*** *average yield of* oxidation of β-citronellol with dioxygen *for 10 QAL independent runs. XFeatureMap: X = Z, ZZ, Pauli. EI: expected improvement. bs: bootstrap resampling for uncertainty quantification.*

QML and QAL have the potential of improving the quality of inferences, making the agent "smarter" – to choose, with higher probability, the next material or synthesis conditions, aiming to enhance their responses, with fewer experiments. QAL is implemented in MLChem4D software.

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References

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