Large Language Model Assisted Optimisation of Photocatalytic Hydrogen Production

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1. Introduction

Bayesian optimisers have been used to assist chemists in the exploration of chemical spaces (Burger et al., 2020). However, they tend to struggle with complex high dimensional spaces. Our previous work demonstrated by providing domain knowledge they can be utilized to work with such problems, which helps to guide the optimiser to search within promising subspaces.(Cissé et al., 2025, 2024)

Herein we demonstrate the utility of using large language models (LLM) to incorporate domain knowledge, performing a closed-loop chemistry experiment using our mobile robotic workflow. As far as the authors are aware, this is the first demonstrated real world experiment with such a high dimensional search space optimised with Bayesian optimisation.

3. Substantial section

The robotic workflow consists of a mobile robot to transfer samples between various stations (see fig 1) to perform photolytic hydrogen production. A python script sets up a server to monitor the progress of the experiment, and to upload the outcome of the experiment to a web application. The web application allows for users to query the results of the experiments and performs the calls to the LLM to reason on the outputs and to suggest logical points for query on the workflow. The web application then downloads the proposed experiment and converts it to a format for the workflow to process and run.

3.1 Related work

Previous experimental work (Burger et al., 2020) was performed with ten-dimension search space with an naïve Bayesian optimiser. Our previous publication regards to the optimiser was demonstrated with various simulated models with up to fifteen-dimension search space.

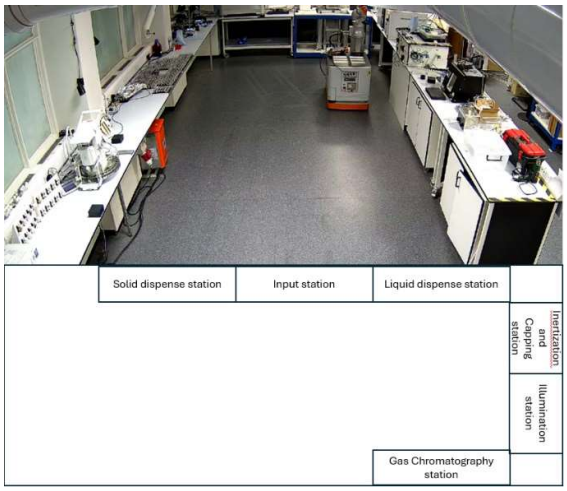

Fig. 1: (Top) Photo of the mobile robotic workflow (Bottom) Layout of the mobile robotic workflow, rotated 90° clockwise with reference to the photo

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