II. Introduction

Bayesian optimization (BO) has emerged as a powerful tool for global optimization of black-box functions, offering a promising approach to efficiently explore the parameter space of complex models. At the heart of BO lies the use of surrogate models and acquisition functions to iteratively refine the search for optimal solutions. This method has been successfully applied across various domains, including materials science, where it has shown remarkable efficiency in identifying optimal material properties [**1**](https://www.nature.com/articles/s41524-021-00656-9).

The advent of bandit algorithms has further enhanced the capabilities of BO by introducing mechanisms for adaptive sampling and decision-making. These algorithms, which operate under uncertainty, have the potential to significantly improve the efficiency of BO by reducing the number of required function evaluations. However, the performance of different bandit algorithms in the context of BO remains an area of active research, with ongoing efforts to benchmark their effectiveness across various experimental domains [**1**](https://www.nature.com/articles/s41524-021-00656-9).

This thesis aims to contribute to the understanding of bandit algorithms within the framework of Bayesian optimization by conducting a comprehensive benchmarking study. The study will evaluate the performance of different bandit algorithms in terms of their ability to efficiently explore the parameter space and converge to optimal solutions. By comparing these algorithms under various experimental conditions, this research seeks to identify the most effective strategies for optimizing decision-making processes in complex, high-dimensional spaces.

The significance of this research lies in its potential to inform the development of more efficient and robust optimization strategies. By providing insights into the performance characteristics of bandit algorithms in Bayesian optimization, this study could guide future research and practical applications in fields such as materials science, machine learning, and engineering, where the ability to efficiently explore and optimize complex models is crucial