Reducing Computational time in 2D Material DFT Simulation with Charge Mixing Optimization via Bayesian Algorithm

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Abstract

This research confronts a pivotal challenge in computational materials science: the elevated computational energy consumption linked with simulating 2D structures through Density Functional Theory (DFT) [1,2]. To address this, our method uses Bayesian optimization, a machine learning method [3], for charge mixing optimization. Our primary objectives encompass the formulation of a systematic methodology that seamlessly integrates Bayesian optimization with DFT simulations for charge-mixing optimization, and an evaluation of its impact on computational efficiency.

In the implementation and fine-tuning of the Bayesian algorithm for optimizing charge mixing parameters in DFT simulations, we focused on the extensively studied graphene as a test case. The outcomes reveal a noteworthy reduction in computational time and convergence rate relative to traditional DFT simulations. Specifically, convergence was achieved after only 12 iterations using the fine-tuned parameters, in contrast to the default settings requiring up to 19 iterations. The Bayesian optimization algorithm adeptly explores the charge mixing parameter space, steering simulations towards swift convergence, and substantially decreasing simulation time, resulting in a time savings of 29% without compromising accuracy.

The integration of Bayesian optimization with DFT not only amplifies materials discovery efficiency but also aligns seamlessly with the imperative for sustainable computational practices.

Keywords: Density Functional Theory (DFT); Bayesian optimization; Charge mixing optimization; Machine learning; Sustainable computational practices

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Figures

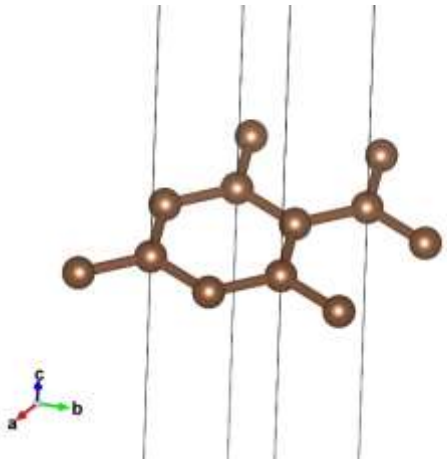

Figure 1. crystal structure of graphene.