Chapter 19
Quantum-Assisted Artificial Intelligence in Chemical Reaction Prediction

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ABSTRACT

Researchers are excited to use these tools to guess reactions that haven't been seen before because they can guess chemical reaction paths, along with the ratios and transition state energy that go with them. Because of this, the methods used to create new ways to use quantum chemical models to guess what reactions will happen are very important. Here are a few examples of how computational methods have been used instead of time-consuming and expensive tests to find new reactions, catalysts, and ways to make complex molecules. Our research also looks at the newest, most cutting-edge methods and possible future developments in this area that is growing very quickly. Our results show that quantum-assisted AI has the ability to completely change the field of computational chemistry, especially when it comes to predicting chemical reactions and making computers faster and smarter.

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INTRODUCTION

Jo 2020 The accurate and efficient forecasting of chemical processes has been a longstanding challenge in the field of chemistry. Traditional computer techniques face a substantial obstacle when dealing with the intricacies of molecular interactions and the vast array of possible reactions. Nevertheless, the fusion of quantum computing and artificial intelligence presents the potential for a groundbreaking transformation in this domain.

Mouchlis 2021 Quantum computing has the capacity to revolutionize our comprehension of chemical systems through its ability to handle vast quantities of data and do computations that are beyond the capabilities of conventional computers. Quantum computers utilize the principles of quantum physics to accurately simulate molecular behavior, offering unprecedented understanding of reaction routes and dynamics. Artificial intelligence approaches, such as neural networks and machine learning, have demonstrated remarkable efficacy in both forecasting events and uncovering patterns in intricate datasets. By integrating AI techniques with quantum computing, the potency of quantum simulations can be enhanced, leading to more precise and efficient chemical reaction prediction.

Gómez-Bombarelli 2018 This research examines the synergistic potential of integrating AI with quantum computing to forecast chemical processes. Firstly, let us examine the constraints and challenges associated with conventional methods of reaction prediction. Subsequently, we will examine AI and quantum computing from a theoretical perspective, drawing comparisons and distinctions between their attributes and advantages. Subsequently, we will explore the potential of combining these two approaches to enhance the precision and scalability of chemical reaction prediction, while simultaneously addressing any preexisting problems.

Christo Ananth 2020 In addition, we examine recent advancements in the domain, such as algorithms influenced by quantum computing and hybrid quantum-classical systems that integrate the most advantageous elements of artificial intelligence. Possible applications of quantum-assisted AI encompass drug discovery, materials investigation, and catalysis, all of which necessitate accurate prediction of chemical reactions. Lastly, we will examine the present state of the discipline, its constraints, and potential avenues for future research and development. This work suggests that the integration of AI with quantum computing has the potential to significantly enhance the accuracy of chemical reaction prediction, hence accelerating advancements in chemical research and its associated disciplines.

How AI Can Be Used in Chemicals

1. Atomwise: Design and Finding New Drugs Atom wise quickly looks through millions of molecules to find possible drug targets by using neural networks that learn from a huge amount of data. This method, which is driven by AI, cuts down on the time needed to make new medicines. Insilico Medicine is a tool that helps make drugs better by using reinforcement learning and generative adversarial networks (GANs) to create new compounds with the right properties.

2. In the field of materials science called citrine informatics, machine learning methods are used to guess what new materials will be like. In order to speed up the process of finding new materials, their platform uses huge libraries with information on how to make materials and describe them. Schwarzinger uses artificial intelligence to guess how chemicals will react and make new materials. Machine learning techniques are used in the programme to run physics simulations.