

Chapter 11

Optimizing Molecular Structures Quantum Computing in Chemical Simulation

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ABSTRACT

Quantum computing has shown promise in chemical simulation and other fields where computationally hard problems must be tackled. This research focuses on optimizing molecule structures, which is an important step in understanding the properties and activities of chemical substances. It also studies the possibility of quantum computing in this domain. The system's many-body wave function is optimized using the imaginary time evolution approach, with nuclei and electrons both being considered quantum mechanical particles. Based on numerical experiments in two-dimensional H_2^+ and $H-C-N$ systems, the authors find that their suggested method may have two benefits—it can find the best nuclear positions with few observations (quantum measurements), and it can find the global minimum structure of nuclei without starting from a complex initial structure and getting stuck in local minima. It is anticipated that this approach would function admirably with quantum computers, and its advancement will pave the road for its potential application as a potent tool.

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INTRODUCTION

Quantum computing is a new technology that has the potential to change many fields, including science. Quantum computing makes it possible to improve molecular structures in chemical modeling in ways that have never been seen before, and it does so very quickly and accurately (Zalka, 1998). This introduction gives a full explanation of why quantum computing is important for chemical modeling and a short summary of the research's main goals and results.

Chemical simulation is a key part of understanding how molecules behave and what their properties are. This helps with drug discovery, materials study, environmental studies, and many other fields. However, traditional computer methods have a lot of problems, especially when working with complicated chemical processes. Quantum phenomena like electron correlation and entanglement are hard for regular computers to correctly copy. These phenomena are very important in chemical reactions.

Using the ideas of quantum physics, quantum computing has the power to solve these problems and change the way chemical models are made. Quantum computers are different from regular computers because they use qubits, which can be entangled and live in more than one state at the same time through superposition. In contrast to traditional computers, which only use bits that are either 0 or 1, this lets them work on a huge number of options at the same time (Ranjit, 2014a).

As the name suggests, this research looks at how quantum computing can be used to improve and speed up computational chemistry methods in order to find the best chemical structures (Christo Ananth, 2015). We are interested in using quantum algorithms, like the variational quantum eigensolver (VQE) and the quantum approximation optimization algorithm (QAOA), to lower the energy of molecular systems and figure out what their basic properties are when they are in their lowest energy state.

Through a thorough review of the relevant research and case studies, we highlight the pros and cons of the current quantum computing approaches used in chemistry modeling. We talk about the problems that noise and mistakes can cause in quantum hardware and different ways to make them less of a problem. We also look at new trends and possible directions in the field, such as the development of error-corrected quantum computers, the use of machine learning techniques in quantum chemistry, and the search for new quantum algorithms that can improve molecular optimization (Combes et al., 1981).

The point of this research is to give you useful information about the amazing things that quantum computing can do in chemical modeling. It also gives researchers and professionals a complete guide on how to use this new technology to speed up scientific progress and discovery in chemistry and related fields.

RELATED WORK

Even though there have been a lot of efforts and progress in recent years, it is still hard to do accurate quantum chemistry calculations on regular computers, especially for molecules that are important in industry. When right methods for quantum chemistry are used on classical computers, the cost of computing goes up exponentially as the molecular size goes up. However, quantum computers can make this cost less by using polynomial scaling. Three calculations in quantum chemistry have been thought to be possible with quantum computers (Kitaev, 1995). By changing the quantum states of matter and using its unique properties, like superposition and entanglement, quantum computers could be used to

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