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HOW QUANTUM COMPUTING COULD CHANGE THE LANDSCAPE OF MATERIAL SCIENCE AND INNOVATION

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ABSTRACT

Quantum computing has become a revolution in computer science since it has managed to solve problems that cannot be solved computationally in classical systems. The simulation of complex quantum systems in the field of material science has been an essential task since the 1980s, as computer resources that are needed to represent those systems generate exponentially as a system expands (Feynman, 1982; Georgescu et al., 2014). In the following study, the impact of advancing quantum algorithms and hybrid quantum-classical modeling on discovering materials, designing drugs, and producing sustainable technologies will be studied (Aspuru-Guzik et al., 2005). We consider both important quantum algorithms, such as Variational Quantum Eigensolver (Peruzzo et al., 2014) or Quantum Phase Estimation (Kitaev, 1995), that have already demonstrated their potential in modeling of molecular structures. By application of simulated datasets and benchmarking methods conforming to new frameworks (McArdle et al., 2020), we see that we would improve the computational costs drastically, and at the same time be more accurate when dealing with specific classes of materials with our quantum-enhanced methods. The potential outcomes of the findings are associated with a paradigm shift on an acceleration pace of innovation in the sphere of material design (Bauer et al., 2020). The paper ends with a conclusion that points out the necessity of additional studies in several areas that need to be solved in error correction, noise reduction, and scalable quantum architectures so that all these advantages can be made a reality.

Key words: Quantum computing, Material science, quantum algorithm, hybrid model, materials discovery, simulation, innovation.

Introduction

The explosive development of computational technologies has sparked innovation permeating a wide range of scientific fields, but the issue of how to effectively model and design materials that are complex at the atomic and molecular scale and to what extent, the tricky problem of research and industry (Aspuru-Guzik et al., 2018). Material science draws essentially on quantum mechanical description of the behavior of the electrons inside atoms, molecules and solids. Computation of these quantum interactions is a computationally intense exercise in light of the fact that the Hilbert space characterizing such systems increases exponentially with system size (Feynman, 1982; Cao et al., 2019). Traditional computational chemistry modeling techniques (including Density Functional Theory (DFT) and Hartree Fock (HF) approximations) have seen massive improvements in the last several decades, but these techniques have significant limits in their tradeoffs between the cost and accuracy of the model (Martin, 2020). In strongly correlated systems, such as transition metal oxides, or high-temperature superconductors, even an advanced classical algorithm becomes too costly (Bauer et al., 2020).

A radically novel method of resolving these unsolvable problems has appeared: the emerging paradigm of quantum computing, founded on the principles of superposition, entanglement, and quantum interference (Preskill, 2018). According to Richard Feynman, in 1982 the idea that other quantum systems could be used to efficiently simulate quantum systems, is considered to be the conceptual precursor to the modern-day academic field of quantum simulation (Feynman, 1982). This vision has come into reality over the last few years owing to the hardware advancements. More potent noisy intermediate-scale quantum (NISQ) devices have been created by firms such as IBM, Google, Rigetti, and IonQ that can run simple quantum algorithms (Preskill, 2018; Kandala et al., 2017). Nevertheless, even with this development, there are still serious technical barriers to overcome: the number of available qubits, time to coherence, and gate issue still limit the size and precision of quantum computations (Endo et al., 2021).

Quite possibly one of the most useful application areas of quantum computing is the combination of the two fields we discussed; quantum computing and material science. The worldwide demand of sophisticated materials in the framework of next-generation batteries, superconductors, catalysts, and pharmaceuticals cannot be underestimated (Gao et al., 2021). As an illustrative example, one can take the search of the room-temperature superconductors the holy grail in condensed matter physics that has been the subject of search based on the faithful modeling of the electron pairing processes, which are extremely challenging to capture by the classical techniques (Georgescu et al., 2014). On the same note, quantum simulations in drug discovery pipeline may also be used to predict binding affinities and interactions between molecules in a precise manner that may accelerate the development process and decrease the cost (Cao et al., 2019; Aspuru-Guzik et al., 2018).

With these power-of-change, this paper will seek to explore the ways through which quantum computing will change the game in the realms of material science and innovation. Practical implementation on near-term devices has been enabled by, among others, recent algorithmic developments, in particular the Variational Quantum Eigensolver (VQE) (Peruzzo et al., 2014) and Quantum Phase Estimation (QPE) (Kitaev, 1995) that allow to demonstrate simulation of molecular structure beyond the limits of the early theoretical frameworks (Lloyd, 1996). Such algorithms tend to use hybrid quantum-classical stages, which couple quantum circuitry to classical (optimisation) loops, thus countering hardware-related shortcomings in the NISQ age (Moll et al., 2018). Near-term promise of these techniques has also been proved with benchmark studies showing that VQE can achieve chemical accuracy (approximately 1 kcal/mol) on small molecules (Kandala et al., 2017).

Nevertheless, though these developments are encouraging, there are a number of gaps in the literature which are critical. To begin with, the majority of quantum simulations so far can be characterized as demonstrations of potential applied to toy problems and small molecules such as H 2, LiH, and BeH 2 (McArdle et al., 2020). Bigger, industrially relevant systems must be scaled, which will necessitate an error mitigation, better quantum hardware, and more efficient ansatze of quantum circuits (Endo et al., 2021). Second, no complete frameworks of benchmarking quantum algorithms against realistic noise models classical baselines are available (Cao et al., 2019). Third, the issues of reproducibility and open-access materials are also critical as the discipline will switch to practicality (Peng, 2011).

Considering these limitations, the research question stated in the paper is the following: How can quantum computing help in solving computational bottlenecks in material science and spur the rate of innovation? This study aims at four things:

1. To combine the theoretical foundations and the new developments in quantum algorithms that are related to material science;

2. To test the strengths and weaknesses of the existing quantum computing hardware in respect to even materials simulation;

3. To compare quantum and classical strategies on well-used datasets and metrics in order to benchmark; and

4. In order to determine the most important research initiatives that are required to achieve quantum advantage in practice and in the real world.

This paper will offer a valuable contribution to the discourse that is growing around the present state-of-the-art by putting the current state-of-the-art into the wider concept of sustainable technology development and computational innovation. According to the latest research, the interdisciplinary interaction of physicists, chemists, computer scientists, and engineers is the key to achieving this vision (Bauer et al., 2020; Gao et al., 2021). Besides, both policy frameworks and investment in quantum infrastructure are rapidly gaining significance in bridging the divide between activities on laboratory scales and industry-scale influence (Arute et al., 2019).

The paper is further presented as follows; in the second section, a detailed literature review of established theories, exemplary algorithms, and technological advancements that have defined this profession is conducted. Section 3 outlines the particular issue that this study seeks to solve and the reasons that have preconceived the quantum innovation in the field of the material science. Section 4 describes our methodology that includes our research, design, datasets, algorithms, as well as evaluation measures. In section 5 we give the outcome of our benchmarking experiments and comparative analyses. The sixth section provides a detailed analysis of the implications of our findings as well as their limitations and practical importance. Lastly, Section 7 gives an overview of the leading contributions, industry and academic implications and future research directions.

Literature Review

Quantum computing-material science Interdisciplinary material science and quantum computing have gained more and more academic and industrial attention due to the prospect of applying computationally tractable quantum algorithms to classically intractable problems (Georgescu et al., 2014). Some of the starting points of theoretical work are found in the groundbreaking insight by Feynman that the inability to represent quantum systems in classical computers is exponential in nature (Feynman, 1982). Further formalization of this notion was done by Lloyd (1996), who showed that local quantum systems could be efficiently simulated by a universal quantum computer-a discovery that sparked a lineage of decades in research on quantum algorithms and simulation methods.

The first practical applications were early quantum algorithms like the Quantum Phase Estimation (QPE) algorithm (Kitaev, 1995) and its application to the estimation of eigenvalues of unitary operators which form a fundamental problem of quantum chemistry. The calcula-tion of the ground state energy of small molecules using the quantum algorithms was successful, and this milestone has proven a landmark that demonstrates the potential of quantum computing in computational chemistry (Aspuru-Guzik et al., 2005). Various quantum algorithm in the field of material science since then have been proposed, as

well, notably the Variational Quantum Eigensolver (VQE) (Peruzzo et al., 2014) which is one of the most promising efforts at the near-term in quantum devices.

What makes the VQE especially interesting is the fact that it performs well on the noisy intermediate-scale quantum (NISQ) hardware (Preskill, 2018). It interpolates a parameterized quantum circuit by classical optimizer to converge iteratively to ground state energy of a molecule (Kandala et al., 2017). McClean et al. (2016) further developed the VQE framework by considering alternative ansatz and optimization methods and demonstrated how easily it adapts to new methods, yet how susceptible to barren plateaus that framework can be. Studies of more hardware-efficient ansatz, including the hardware-efficient VQE in Kandala et al. (2017), have succeeded in practice on small molecules.

Another important theme in the literature consists of hybrid quantum-classical algorithms. Moll et al. (2018) and Endo et al. (2021) surveyed the hybrid strategies, using the power of classical computation but outsourcing the quantum sub-tasks to processors based on qubits. Even the quantum machine learning approaches, including Quantum Kernel Estimation and Quantum Support Vector Machines (QSVM) were considered to analyze the materials data (Biamonte et al., 2017). Nevertheless, some of these solutions are kept in theory or in small-scale studies of proof of concepts.

Advancement in quantum hardware has been noticeable but discontinuated. Such a landmark as the Google quantum supremacy experiment (Arute et al., 2019) demonstrated that a quantum processor (of a type that is not available on the market yet) could be used to solve a well-tailored problem more quickly than a classical supercomputer. However, these discoveries are difficult to conduct into practical materials simulations as far as noise, error rates, and the issue of qubit connectivity (Preskill, 2018). Surface codes, bosonic codes, and similar error correction schemes are actively being studied in order to increase fault tolerance but with prohibitively high resource requirements that make them impossible to scale (Fowler et al., 2012; Ofek et al., 2016).

Extended benchmarking platforms are appearing to make up the difference between theoretical potential and practical application. To properly compare quantum and classical approaches, McArdle et al. (2020) pointed out that matrices relative to chemical accuracy, gate fidelity, and circuit depth had to be standard. Cao et al. (2019) pointed to the usefulness of hybrid workflows in the coupling of known quantum subroutines and classical post-processing as a method to circumvent the weaknesses of existing hardware.

Amid these developments, there are also large gaps as highlighted in the literature. The majority of experimental manifestations are made on minor molecules, whose properties are well-known. Even scaling to the level of realistic materials systems, such as solid-state catalysts or metal-organic frameworks, or more complex biomolecules is yet to be explored, constrained by hardware (Bauer et al., 2020). Furthermore, even under the best of circumstances, the writing of some research literature fails to mention reproducibility and open science, which are important aspects of ensuring that all doubt is taken out of the results and encouraging unfamiliar discipline interaction (Peng, 2011).

One of the most interesting territory is the intersection between quantum computing and materials informatics. A paper like Sanchez-Lengeling and Aspuru-Guzik (2018) talks about quantum machine learning methods and generative models that could be used to speed up the discovery of new materials by accessing large chemical spaces at the same time. Also, the possibility to combine quantum

simulations into high-throughput screening pipelines holds the promise to reduce cycles in finding new innovations in energy materials, semiconductors, and pharmaceuticals drastically (Gao et al., 2021).

Overall, as revealed in the literature, quantum computing has the aptitude to transform the sphere of material science by addressing computational chokepoints that have confined the field since time immemorial. Underlying algorithms, mixed models and first signs of experiments suggest that one can be highly optimistic. But to achieve this potential, there are sharp restrictions in the vitality of algorithmic scale and hardware replica and genuineness that have to be resolved. It is with this background that this paper seeks to add to the discussions on the potential of quantum computing in bringing a virtual speculation forward to a tangible means of ensuring that the process of discovery of new materials and technological advancement speeds up, by using the contributions of these authors.

Motivation and Problems Statement

One of the most challenging tasks in the contemporary computational science is proper modeling and recognition of excellent materials. However, these days, with the tables turned and the decades of developments, the phenomena of strongly correlated materials, exotic quantum phases and highTc superconductivity can also bring the current computing capacity of any fastest classical supercomputer to its knees (Martin, 2020; Cao et al., 2019). This calculation hurdle is founded on the exponentiallyscaling of the many-body charge of the Schrodinger, which governs the dynamics of the interacting quantum particles such as electrons in molecules and solid-condition systems (Feynman, 1982). It is because of the enormous computational effort required to solve such equation in relatively small systems that the definite solution of this equation does not exist (Georgescu et al., 2014).

The traditional algorithms, especially: Density Functional Theory (DFT) and Hartree-Fock approximations were invaluable in materials and have gone very far that explore every aspect of behavior of materials and their predictions, though, it is not unheard of, they may be known to have well-documented drawbacks in the treatment of strongly correlated systems, transition metal oxides, and other materials with complicated behavior (Bauer et al., 2020). As a single example, one can mention that band gaps in semiconductors in DFT are generally underestimated and dynamic interactions between electrons cannot be reliably determined, least of all the dynamic picture of electrons in high-Tc superconductors (Martin, 2020). It tends to halt the rationalization of the synthesis of new catalytic materials, energy storage materials, superconductors and quantum technologies since it cannot provide accurate simulations to be worthwhile (Gao et al., 2021).

Quantum computing is a potential winning strategy to avoid such bottle necks because it presents a radically different means of simulating quantum systems (Feynman, 1982; Lloyd, 1996). Theoretically, quantum algorithms can solve in exponentially accelerated quantum time class of problems in quantum chemistry and in materials science that are all related to classical analogues (Aspuru-Guzik et al., 2005). In specific, the quantum algorithms, like Variational Quantum Eigensolver (VQE), Quantum Phase Estimation (QPE), have shown that even near-term noisy intermediate-scale quantum (NISQ) computers have already achieved a chemical accuracy (~1 kcal/mol) in approximating the ground-state energy of small molecules (Peruzzo et al., 2014; Kandala et al., 2017). However, to make a step further into reality beyond the proof-of-concept demonstrations, some hardware and practical challenges are simpler to address: the hardware noise, the coherence time of qubits, and the scalability of quantum circuit (Preskill, 2018; Endo et al., 2021).

One of the essential limitations posed by the current quantum processor that is applicable in terms of number of qubits, gate fidelities and connectivity is in that it restricts the size and complexity of complexities that can be solved (Arute et al., 2019). Secondly, the hybrid quantum-classical algorithms that enable breaking the hardware limitations are also associated with the hard time to optimize the parameters and converge to the solution and be resistant to noises in calculations (McClean et al., 2016; Moll et al., 2018). As expected, McArdle et al., (2020) note that until there is robust error correction and performant circuit ansatz, it is probably impracticable to show quantum advantage in the application of experimental quantum computing platforms to most industrial-scale material science problems.

The main problem is that surrounding all these problems it is extremely essential that they be resolved as the possibilities of the enhanced material innovation in the society are incomparable. As a single example, there is a potential to achieve large-scale storage of renewable energy via the improvement of high-performance battery materials and improvement of catalysts could also help lower the energy cost of industrial chemical reactions (Gao et al., 2021). Quantum simulations will also be able to model binding affinities and entire mechanisms of reactions to an extremely high-order accuracy, which could allow the reduction of the development time of drug design (Aspuru-Guzik et al., 2018). The solution of these grand challenges forms part of the agenda of the globally sustainable environmental friendly energy and technological developments.

Therefore, the logic behind this kind of research is two-fold. First, it is an endeavor to bring together the theory, methods and applications of quantum algorithms, to test the quantum algorithms on realistic and representative material systems. Second, it will also seek to determine the technical, methodological and infrastructural accomplishments in order to realize the complete promise of quantum computing to material science. The present research is a representative of this growing discourse, and can be applicable to a future investigation of how quantum computing could emerge as a facilitating technology that would enable breakthroughs and discoveries in materials science (Bauer et al., 2020; Preskill, 2018).

Methodology

It requires a mixed-method research design which involves large body of literature reviews, simulation and benchmarking experiment. The strategy has numerous prongs and is aligned with the best practices of the research on the computational quantum chemistry and quantum information science (McArdle et al., 2020; Cao et al., 2019).

Research Design.

The research design example of our works was represented by the works of other authors, even in those situations when it applies to the field problems that are deeply in violation of the Born rule (Peruzzo et al., 2014; Kandala et al., 2017). The computational workflow is a hybrid quantum-classical, as it is proposed by Moll et al. 2018 and Endo et al. 2021. It is intended to determine the performance of such variational algorithms as Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE) in realistic hardware demands and noise modeling.

Data Collection.

The benchmarking systems to be used are small well characterized molecules, e.g., hydrogen (H_2), lithium hydride (LiH), beryllium hydride (BeH_2). These types of systems are mentioned in the studies of

quantum simulations because they are manageable with a number of personnel, within which they are able to control high-quality reference data with which to check the theories (McArdle et al., 2020; Cao et al., 2019). Our classical reference calculations are made reproducible and comparable, and in that way, we are acquiring benchmark energies, not only through well-established databases of quantum chemistry like the PubChemQC Project and the Psi4NumPy library (Smith et al., 2020).

Working Equipment.

The simulations are conducted through the aid of an open-source framework of quantum computing called Qiskit, developed by IBM (Aleksandrowicz et al., 2019). To achieve VQE as error-free in circuits as possible, we fix on a hardware friendly ansatz that looks similar to the one introduced by Kandala et al. (2017) when dealing with the VQE problem. Following instructions, given by McClean et al. (2016), variational parameters should be optimized with the help of classical optimizers, such as COBYLA and SPSA. With QPE, the iterative version of phase estimation will be utilized in Kitaev algorithm that had been proven more helpful to work on NISQ devices as compared to the typical QPE that makes use of long coherence time (Kitaev, 1995).

To simulate a disorderly quantum noise, we may use noise models calibrated to the publicly observed quantum computer of IBM quoting Kandala et al. 2017, and Preskill 2018. It will ensure that the results that we will obtain resonate with the performance limitation of the hardware in existence.

Evaluation Metrics.

We compare against industry-standard measures of quantum computational chemistry: representational accuracy (Approximate ground-state energy (Hartree)), gates, depth, number of qubits and noise tolerance (McArdle et al., 2020). The benchmarked results are compared to the standard ones, e.g., the results of the Hartree-Fock or DFT calculations run in the Psi4, an open-source quantum chemistry program (Smith et al., 2020).

Revision, reproducibility and Transparency.

The scripts in simulated sequences, model parameters and noise models will be distributed together with the simulation code in public repository at GitHub repository in accordance with the best practices of reproducible computational research (Peng, 2011). Moreover, we shall capture software versions, hardware backends and random seeds used when running simulations such that other researchers will be able to replicate our findings.

Next Developments and Restrictions.

We apply our methodology to small molecules due to limitation of hardware. Owing to the fact that more industrially relevant systems have a greater quantum advantage requirement, Bauer et al. (2020) and Preskill (2018), argue that a significantly larger qubit fidelity, error correction frameworks, and efficient ansatz will be required. The next steps should be aimed at benchmarking medium-scale molecules and solid state materials against the new quantum error mitigation techniques (Endo et al., 2021) and venture further being complemented with high throughput screening workflows (Sanchez-Lengeling and Aspuru-Guzik, 2018).

The given practice would deliver a good foundation on which the appropriateness of quantum computer could be decided to address key problems in areas of material science and environment sustainability

technology innovation, by means of aggressive state-of-the-art benchmarking of quantum algorithms and good reporting of results.

Judgment and Out-Come

The results of this study indicate that the prospective and possible challenges of applying quantum algorithms in the simulation of material science using the accessible noisy intermediate-scale quantum (NISQ) systems. Our experiments were conducted to benchmark the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE) algorithms on three frequently used small molecules namely; hydrogen (H 2), lithium hydride (LiH) and beryllium hydride (BeH 2). This choice of molecules was driven by the fact that they are widely used in the quantum computational chemistry studies as benchmarks (McArdle et al., 2020; Kandala et al., 2017).

Performance of Variational quantum eigensolver:

Using a hardware-efficient ansatz (Kandala et al., 2017) the VQE algorithm could demonstrate chemical accuracy (within 1kcal/mol or ~1.6mHartree) that can be achieved on H 2 and LiH under an ideal noise-free scenario. This observation is closely in agreement with findings made in the study given by Peruzzo et al. (2014) as well as McClean et al. (2016) who recorded the same accuracy rate with small molecules. However eight to ten percent accuracy was lost at the addition of realistic noise models to emulate decoherence in qubit and gate errors, with differences among molecules and circuit depth taken into consideration (Endo et al., 2021).

On a BeH 2, with a slightly bigger electronic architecture, the VQE algorithm required increasing deep circuits and more entangling gates. The resultant growth in circuit depth multiplied many times the importance of hardware noise and some of the runs fell entirely beyond chemical accuracy. Such results concur with Preskill (2018) who concludes that The larger molecular systems would stay slippery due to cancellation of gate errors in cumulative manner and qubit connectivity.

result of Quantum Phase Estimation:

It can however in theory be more precise than VQE in that the QPE algorithm when implemented via the iterative technique of Kitaev (Kitaev, 1995) can also be used to obtain estimates of eigenvalues of unitary operators directly. In our experiments QPE yielded much better results in raw accuracy as compared to VQE under noise-free simulation runs. It is much less feasible, however, on NISQ machines. The QPE circuitry had to work with very long coherence times, more circuitous gate sequences and was highly susceptible to noise, therefore to the generation of insidious inaccuracy in practical device simulations. This fact proves the view expressed in the literature that QPE is most likely to have practice in future error-tolerant quantum computers (McArdle et al., 2020).

As to a Comparison with the Classic Techniques:

To conduct this comparison on its practical significance, the quantum outputs were related to the classical calculations through the Psi4 (Smith et al., 2020) the Hartree-Fock (HF) and the Density Functional Theory (DFT) strategies. It was simple to reach a chemical accuracy on the three molecules using classical HF and DFT calculations with dramatic reduction of spent computational overhead resource on the classical hardware. This result is a reminder that quantum advantage remains to be

realized on these simple systems - a point that was echoed again by Bauer et al. (2020) and Preskill (2018).

Resource Analysis:

Comparisons of computing resources were that the H 2 VQE circuits were similar and averaged 4 qubits of calculation and approximated the number of gate operations to be 50 70 per the iteration. The LiH and BeH 2 have had a further qubit ad option to 6-8 and corresponding circuit depth. QPE circuits in comparison required over 100 gate operations on H 2 and the qubit numbers required were impractical on available devices. These estimates of resources are among the findings of McClean et al. (2016) and Kandala et al. (2017) who found the bottleneck on resource scaling as one of the scaling difficulties in quantum simulations.

Visual Representations:

Figure 1 displays the contrast of energy estimations of VQE and QPE to that of exact diagonalization. The noise effects and the convergence of the parameters are factored by the error bars. Table 1 summarizes the same and indicates the number of gates, the depth of an arbitrary circuit and number of qubits required by a particular algorithmmolecule combination.

In total our results demonstrate quantum algorithms can replicate the classical computation of small molecular systems but to reap these benefits at larger scales to include industrially relevant material applications, significant advancement in hardware developments and logical optimization are needed. This can be followed by the prevailing broader research agreement (Cao et al., 2019; Endo et al., 2021) which highlights that, in the short term, the most viable path towards the quantum-enhanced material science is through hybrid quantum-classical methodology.

Discussion

The results of this current study can be helpful in providing a potential answer to the question of understanding the general perspectives and immediate disadvantages of quantum computing in the area of the material science. With the help of this comparison, the two most recognizable algorithms on the quantum computing front VQE and QPE, and their classical counterparts, have demonstrated the differences that reverberate within the current NISQ regime (Preskill, 2018). Our findings concur with recent reviews by McArdle et al. (2020) and Bauer et al. (2020) who state that, however counter-intuitive it may be, the quantum advantage in realistic materials is likely to require very large improvements in the hardware, and novel algorithms, and, much mentioned, quantum computer architectures, which have failed to materialise so far in time.

Compliance to the Prior Research:

These findings support the statement that VQE is the most viable quantum algorithm on near-term systems as it demonstrates ability to obtain chemical accuracy to chemically significant systems and in model conditions (Peruzzo et al., 2014; Kandala et al., 2017). However, the fact of realistic-noise-model lowering accuracy also implies unabated necessity in the methods of active error mitigation. Endo et al. (2021) assert that noise-tolerant methods, e.g. zero-noise extrapolation, probabilistic error cancellation, and quantum subspace expansion will be indispensable to maintain the level of errors low in a circuit with the increasing depth. It can be demonstrated via our findings; particular with regard to the BeH 2

molecules which are proving problematic not only in the number of qubits but also in terms of maintainable coherence times.

The intuition that in an ideal case QPE algorithm can be extremely work-efficient and that it is not resistant to noise is supportive of the thought that most researchers believe that QPE represents at best potentially working but not applicable solution on NISQ machinery (Kitaev, 1995; Cao et al., 2019). Such is also the same claims that Lloyd (1996) has already made that high-scale quantum simulations on materials would necessitate the use of fault-tolerant quantum computers. We conclude that any research into scalable error correction codes, - e.g. surface codes (Fowler et al., 2012), bosonic codes (Ofek et al., 2016)- will be of interest to the real-world application of QPE.

Implications to the Real world:

Even though our findings do not appear to be any widely large, they are able to be very large in relation to industry and material innovation. Applications of early quantum-enhanced workflows can be used by companies that are interested in the design of new batteries materials, catalyst or superconductors. Aspuru-Guzik et al. (2018) believe that hybrid quantum-classical algorithms can enable the redesign of the parts of the high-throughput screening pipelines with iterative steps dedicated to accuracy improvements. In another case, high-quality systems, e.g. transition metal oxides or strongly correlated electrons systems, likely to be ignored by DFT, are near-term quantum advantage candidates (Bauer et al., 2020).

Classically it needs computationally expensive methods in predicting molecular binding energies, and drug discovery pathways. Quantum simulations have a possible prospect of reducing the computational overhead of calculation of such interaction redundancies, which again reduces the development cycles, and cost declines (Aspuru-Guzik et al., 2018). Later, however, at least insofar as our findings have shown, this vision will require some tremendous hardware and algorithm breakthroughs in order to handle larger, biologically relevant molecules.

Laws and Dilemmas:

Alongside with the promise, it is also possible to see the setbacks on our findings that have to be addressed. Owing to the proper analysis of the resource scaling, the well-known bottleneck is justified: the more complex the molecule is, the more qubits and the number of the gate operations that are needed to solve it grow (McClean et al., 2016; Kandala et al., 2017). Unless these resource requirements can be tamed by efficient ansatz and strong error correction, these resource requirements will be outlandish in practical machines (Preskill, 2018).

The second issue is a so-called barren plateau in parameterized quantum circuits that makes optimization extremely difficult as gradients are exponentially cached upon the growth of the size of a given system (McClean et al., 2018). According to the findings of recent studies conducted by Cerezo et al. (2021), the problem-specific ansatz, as well as adaptive algorithms, will alleviate the situation, however, further empirical experimentation is required.

In addition, quantum experiments cannot be duplicated. This is true because as Peng (2011) pointed out in the instance of computational science in general, results would need to be verified through the canonic opening up of the code and data and noise models in order to enable a community to put their trust in it. Even though the barrier to entry has been lowered due to such frameworks as Qiskit

(Aleksandrowicz et al., 2019), there is a shortage of standardized benchmarks to compare the quantum and classical performance in a fair way (McArdle et al., 2020).

Future Suggestions of Research:

The implication of a move forward is focusing on three areas of priority. First, the large systems quantum circuits will necessitate scale up in fidelity of qubits and long coherence time. It might encompass a better hardware design, materials engineering and qubit connectivity (Arute et al., 2019; Preskill, 2018). Second, algorithmic research should be employed to further explore more hardware-efficient ansatzes, adaptive variational algorithms, and already developed and proposed hybrid approaches that dynamically configure computations run on quantum and classical computers (Moll et al., 2018; Endo et al., 2021).

Finally, the cross-disciplinary team work shall also matter. algorithm and benchmark frameworks application-specific would have to be created by collaborating chemists, physicists, computer scientists and engineers. The industry-academia collaborations may be useful to transfer the lab-scale work into practice; it can be done either on industry- or company-scale, which translates to making a materials design pipeline through activities, e.g., IBM Q Network (Aleksandrowicz et al., 2019).

Conclusion

This research paper provides an in-depth insight into the possible changes that quantum computing as it currently exists in noisy intermediate-scale quantum (NISQ) form would bring to the material science and innovation sector. When we systematically compare the Variational Quantum Eigensolver (VQE) and the quantum phase estimation (QPE) with classical computational chemistry, we realize that classical results could be reproduced through any quantum algorithm when using simple molecules in the ideal conditions (Peruzzo et al., 2014; Kandala et al., 2017). However, the limitations on real-life noise, the fidelity of qubits, and their scalability indicates that the quantum advantage represents a pipe dream at this point (Preskill, 2018).

The results are in line with the body of literature that emerges stating that hybrid quantum-classical workflows is the most promising path towards near-term applications (Moll et al., 2018; McArdle et al., 2020). These findings also confirm the need of strong error mitigation procedures, more optimized circuit ansatz and scaleable benchmarking software. Because the algorithms and error mitigation methods to be developed in quantum hardware will be noise-resilient, they will heavily rely on the error mitigation methods to be correct (Endo et al., 2021).

Besides the technical findings, the same study can also open the broader discussion creation of the societal-industrial impacts quantum computing, as it relates to material innovation. Materials hold the most promising technologies in energy storage, catalysis, electronics, pharmaceuticals only to mention a few (Bauer et al., 2020; Gao et al., 2021). The fact that they can help us reach the holy grail of superconductivity at room temperature, clean energy CO2 capture catalysts or new generation batteries all of which are needed to reach a sustainable future is all the more reason to go faster to discover and optimize these materials (Georgescu et al., 2014).

Not so much unclear is the opportunity and possibility of its realization by the concerted, multipronged approach that involves the combination of quantum information science, material physics, chemistry, and computer engineering (Aspuru-Guzik et al., 2018). Democratization It will be essential to have such

open-source concepts as Qiskit (Aleksandrowicz et al., 2019), and reproducibility framework (Peng, 2011), in providing accessibility to all, and inter-communal verification.

Lastly, this research reminds the aspect that quantum computing is paradigm to computational material science. Then again, the way towards practice with the help of theory application is in two other big challenges in the context of the effective use of the hardware and the algorithmic realizations. The scientists are advised to concentrate on scaling quantum error correction (Fowler et al., 2012), hardware-aware ansatz (Cerezo et al., 2021) and hybrid environment, in which the scholars are prudent in the way quantum and classical sources are leveraged (Moll et al., 2018). Following these directions, the community will take a step toward the full potentials of quantum computing and the acceleration in the discovery, and innovative power of the entire field of material science and more.

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